

Diisoamyl ether

Other names:	1-isopentyloxy-3-methylbutane 2,8-dimethyl-5-oxanonane Butane, 1,1'-oxybis[3-methyl- DI-ISOPENTYL ETHER Di-3-methylbutyl ether Diisopentyl ether Isoamyl ether Isoamyl oxide Isopentyl ether NSC 9281 bis(3-methylbutyl) ether bis(3-methylbutyl)ether di-(3-methylbutyl) ether ether, diisoamyl ether, diisopentyl
Inchi:	InChI=1S/C10H22O/c1-9(2)5-7-11-8-6-10(3)4/h9-10H,5-8H2,1-4H3
InchiKey:	AQZGPSLYZOOYQP-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CC(C)CCOCCC(C)C
Mol. weight [g/mol]:	158.28
CAS:	544-01-4

Physical Properties

Property code	Value	Unit	Source
gf	-76.56	kJ/mol	Joback Method
hf	-392.51	kJ/mol	Joback Method
hfus	15.80	kJ/mol	Joback Method
hvap	51.40	kJ/mol	NIST Webbook
hvap	49.94	kJ/mol	NIST Webbook
log10ws	-2.61		Crippen Method
logp	3.095		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpole	999.00		NIST Webbook
rinpole	1000.00		NIST Webbook
rinpole	987.00		NIST Webbook
rinpole	988.00		NIST Webbook

rinpol	980.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1067.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1063.00		NIST Webbook
tb	445.80 ± 0.50	K	NIST Webbook
tb	445.70	K	NIST Webbook
tb	446.40 ± 0.50	K	NIST Webbook
tb	446.50 ± 0.35	K	NIST Webbook
tb	444.00 ± 4.00	K	NIST Webbook
tc	619.25	K	Joback Method
tf	194.69	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.48	J/molxK	449.74	Joback Method
cpg	358.04	J/molxK	477.99	Joback Method
cpg	373.04	J/molxK	506.24	Joback Method
cpg	387.51	J/molxK	534.50	Joback Method
cpg	401.45	J/molxK	562.75	Joback Method
cpg	414.87	J/molxK	591.00	Joback Method
cpg	427.77	J/molxK	619.25	Joback Method
dvisc	0.0033142	Paxs	237.20	Joback Method
dvisc	0.0125876	Paxs	194.69	Joback Method
dvisc	0.0013091	Paxs	279.71	Joback Method
dvisc	0.0006607	Paxs	322.22	Joback Method
dvisc	0.0003911	Paxs	364.72	Joback Method
dvisc	0.0002583	Paxs	407.23	Joback Method
dvisc	0.0001845	Paxs	449.74	Joback Method
hvapt	47.60	kJ/mol	369.00	NIST Webbook
hvapt	41.40	kJ/mol	443.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54424e+01
Coeff. B	-4.12026e+03
Coeff. C	-6.50410e+01
Temperature range (K), min.	336.92
Temperature range (K), max.	471.74

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	2.00294e+02
Coeff. B	-1.37408e+04
Coeff. C	-2.77392e+01
Coeff. D	2.18467e-05
Temperature range (K), min.	287.15
Temperature range (K), max.	433.15

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
283.15	100.00	782.76

288.15	100.00	778.71
293.15	100.00	774.66
298.15	100.00	770.6
303.15	100.00	766.54
308.15	100.00	762.46
313.15	100.00	758.37
318.15	100.00	754.27
323.15	100.00	750.16
328.15	100.00	746.03
333.15	100.00	741.88
283.15	5000.00	786.88
288.15	5000.00	782.95
293.15	5000.00	779.03
298.15	5000.00	775.09
303.15	5000.00	771.15
308.15	5000.00	767.21
313.15	5000.00	763.24
318.15	5000.00	759.27
323.15	5000.00	755.32
328.15	5000.00	751.35
333.15	5000.00	747.34
283.15	10000.00	790.71
288.15	10000.00	786.89
293.15	10000.00	783.04
298.15	10000.00	779.24
303.15	10000.00	775.41
308.15	10000.00	771.57
313.15	10000.00	767.74
318.15	10000.00	763.91
323.15	10000.00	760.1
328.15	10000.00	756.23
333.15	10000.00	752.39
283.15	15000.00	794.36
288.15	15000.00	790.64
293.15	15000.00	786.89
298.15	15000.00	783.18
303.15	15000.00	779.46
308.15	15000.00	775.74
313.15	15000.00	772.01
318.15	15000.00	768.28
323.15	15000.00	764.59
328.15	15000.00	760.85
333.15	15000.00	757.12
283.15	20000.00	797.85

288.15	20000.00	794.22
293.15	20000.00	790.55
298.15	20000.00	786.94
303.15	20000.00	783.3
308.15	20000.00	779.67
313.15	20000.00	776.05
318.15	20000.00	772.42
323.15	20000.00	768.84
328.15	20000.00	765.22
333.15	20000.00	761.58
283.15	25000.00	801.22
288.15	25000.00	797.65
293.15	25000.00	794.08
298.15	25000.00	790.54
303.15	25000.00	786.98
308.15	25000.00	783.45
313.15	25000.00	779.9
318.15	25000.00	776.38
323.15	25000.00	772.87
328.15	25000.00	769.33
333.15	25000.00	765.79
283.15	30000.00	804.45
288.15	30000.00	800.95
293.15	30000.00	797.46
298.15	30000.00	793.99
303.15	30000.00	790.53
308.15	30000.00	787.05
313.15	30000.00	783.59
318.15	30000.00	780.14
323.15	30000.00	776.74
328.15	30000.00	773.28
333.15	30000.00	769.84
283.15	35000.00	807.58
288.15	35000.00	804.15
293.15	35000.00	800.71
298.15	35000.00	797.31
303.15	35000.00	793.91
308.15	35000.00	790.52
313.15	35000.00	787.12
318.15	35000.00	783.75
323.15	35000.00	780.43
328.15	35000.00	777.06
333.15	35000.00	773.7
283.15	40000.00	810.61

288.15	40000.00	807.23
293.15	40000.00	803.86
298.15	40000.00	800.51
303.15	40000.00	797.19
308.15	40000.00	793.86
313.15	40000.00	790.53
318.15	40000.00	787.22
323.15	40000.00	783.97
328.15	40000.00	780.66
333.15	40000.00	777.39
283.15	45000.00	813.52
288.15	45000.00	810.19
293.15	45000.00	806.9
298.15	45000.00	803.61
303.15	45000.00	800.34
308.15	45000.00	797.07
313.15	45000.00	793.81
318.15	45000.00	790.57
323.15	45000.00	787.37
328.15	45000.00	784.15
333.15	45000.00	780.93
283.15	50000.00	816.37
288.15	50000.00	813.09
293.15	50000.00	809.84
298.15	50000.00	806.62
303.15	50000.00	803.4
308.15	50000.00	800.19
313.15	50000.00	796.97
318.15	50000.00	793.81
323.15	50000.00	790.66
328.15	50000.00	787.49
333.15	50000.00	784.33
283.15	55000.00	819.14
288.15	55000.00	815.91
293.15	55000.00	812.71
298.15	55000.00	809.51
303.15	55000.00	806.36
308.15	55000.00	803.2
313.15	55000.00	800.03
318.15	55000.00	796.91
323.15	55000.00	793.83
328.15	55000.00	790.7
333.15	55000.00	787.59
283.15	60000.00	821.82

288.15	60000.00	818.64
293.15	60000.00	815.48
298.15	60000.00	812.33
303.15	60000.00	809.23
308.15	60000.00	806.11
313.15	60000.00	803.0
318.15	60000.00	799.93
323.15	60000.00	796.89
328.15	60000.00	793.83
333.15	60000.00	790.76
283.15	65000.00	824.44
288.15	65000.00	821.33
293.15	65000.00	818.18
298.15	65000.00	815.07
303.15	65000.00	812.01
308.15	65000.00	808.94
313.15	65000.00	805.88
318.15	65000.00	802.85
323.15	65000.00	799.86
328.15	65000.00	796.84
333.15	65000.00	793.83

Reference

<https://www.doi.org/10.1016/j.fluid.2016.02.009>

Sources

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Legend

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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