

2-Heptanol, 3-methyl-

Other names:	3-Methyl-2-heptanol
Inchi:	InChI=1S/C8H18O/c1-4-5-6-7(2)8(3)9/h7-9H,4-6H2,1-3H3
InchiKey:	SZERMVMTUUAYML-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(C)C(C)O
Mol. weight [g/mol]:	130.23
CAS:	31367-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-1.72		Aqueous Solubility Prediction Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	439.25 ± 0.50	K	NIST Webbook
tb	439.30	K	NIST Webbook
tb	445.65 ± 3.00	K	NIST Webbook
tc	639.93	K	Joback Method
tf	210.74	K	Joback Method
vc	0.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.39	J/mol×K	473.74	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method
cpg	314.22	J/mol×K	529.14	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method

cpg	346.54	J/mol×K	612.23	Joback Method
cpg	356.45	J/mol×K	639.93	Joback Method
cpl	297.50	J/mol×K	298.50	NIST Webbook
dvisc	0.3001577	Paxs	210.74	Joback Method
dvisc	0.0290327	Paxs	254.57	Joback Method
dvisc	0.0055777	Paxs	298.41	Joback Method
dvisc	0.0016351	Paxs	342.24	Joback Method
dvisc	0.0006333	Paxs	386.07	Joback Method
dvisc	0.0002977	Paxs	429.91	Joback Method
dvisc	0.0001609	Paxs	473.74	Joback Method
hvapt	48.00	kJ/mol	390.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.74676e+01
Coeff. B	-5.66044e+03
Coeff. C	1.22600e+00
Temperature range (K), min.	328.25
Temperature range (K), max.	464.42

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31367461&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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