

1-Heptanol, 3-methyl-

Other names:	3-Methyl-1-heptanol 3-Methylheptanol
Inchi:	InChI=1S/C8H18O/c1-3-4-5-8(2)6-7-9/h8-9H,3-7H2,1-2H3
InchiKey:	MUPPEBVXFKNMCI-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(C)CCO
Mol. weight [g/mol]:	130.23
CAS:	1070-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-122.78	kJ/mol	Joback Method
hf	-365.96	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	49.69	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.195		Crippen Method
mvol	129.450	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
tb	458.95 ± 0.50	K	NIST Webbook
tc	637.10	K	Joback Method
tf	225.74	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.23	J/mol×K	474.18	Joback Method
cpg	302.08	J/mol×K	501.33	Joback Method
cpg	313.47	J/mol×K	528.49	Joback Method
cpg	324.43	J/mol×K	555.64	Joback Method
cpg	334.96	J/mol×K	582.79	Joback Method

cpg	345.08	J/mol×K	609.94	Joback Method
cpg	354.79	J/mol×K	637.10	Joback Method
dvisc	0.1178389	Paxs	225.74	Joback Method
dvisc	0.0169844	Paxs	267.15	Joback Method
dvisc	0.0041171	Paxs	308.55	Joback Method
dvisc	0.0013956	Paxs	349.96	Joback Method
dvisc	0.0005948	Paxs	391.37	Joback Method
dvisc	0.0002984	Paxs	432.77	Joback Method
dvisc	0.0001689	Paxs	474.18	Joback Method
hvapt	53.40	kJ/mol	409.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.70207e+01
Coeff. B	-5.32992e+03
Coeff. C	-2.92000e+01
Temperature range (K), min.	347.73
Temperature range (K), max.	484.39

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1070322&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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