3-Heptanol, 3-methyl-

Other names: 2-Ethyl-2-hexanol
3-Methyl-3-heptanol
Inchi: InChI=1S/C8H18O/c1-4-6-7-8(3,9)5-2/h9H,4-7H2,1-3H3
InchiKey: PQOSNJHBSNZITJ-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCCCC(C)(O)CC
Mol. weight [g/mol]: 130.23
CAS: 5582-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-117.50	kJ/mol	Joback Method
hf	-369.43	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-1.60		Estimated Solubility Method
log10ws	-1.60		Aqueous Solubility Prediction Method
logp	2.338		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1019.00		NIST Webbook
rinpol	1010.00		NIST Webbook
tb	436.65 ± 3.00	K	NIST Webbook
tb	432.55 ± 0.70	K	NIST Webbook
tb	443.00 ± 4.00	K	NIST Webbook
tb	436.05 ± 0.50	K	NIST Webbook
tc	640.25	K	Joback Method
tf	243.16	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	349.91	J/mol×K	612.10	Joback Method
cpg	359.77	J/mol×K	640.25	Joback Method
cpg	292.85	J/mol×K	471.39	Joback Method
cpg	305.37	J/mol×K	499.53	Joback Method
cpg	317.32	J/mol×K	527.68	Joback Method
cpg	328.71	J/mol×K	555.82	Joback Method
cpg	339.57	J/mol×K	583.96	Joback Method
dvisc	0.0001803	Pa×s	471.39	Joback Method
dvisc	0.0003166	Pa×s	433.35	Joback Method
dvisc	0.0742698	Pa×s	243.16	Joback Method
dvisc	0.0138116	Pa×s	281.20	Joback Method
dvisc	0.0038351	Pa×s	319.24	Joback Method
dvisc	0.0013989	Pa×s	357.27	Joback Method
dvisc	0.0006196	Pa×s	395.31	Joback Method
hvapt	54.70	kJ/mol	385.50	NIST Webbook
hvapt	54.10	kJ/mol	388.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41942e+01
Coeff. B	-3.26126e+03
Coeff. C	-1.02431e+02
Temperature range (K), min.	336.94
Temperature range (K), max.	469.58

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5582821&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/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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