3-Heptanol, 5-methyl-

Other names: 5-Methyl-3-heptanol
5-methylheptan-3-ol
Inchi: InChI=1S/C8H18O/c1-4-7(3)6-8(9)5-2/h7-9H,4-6H2,1-3H3
InchiKey: SECKOSOTZOBWEI-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCC(C)CC(O)CC
Mol. weight [g/mol]: 130.23
CAS: 18720-65-5

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	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	944.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	942.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1296.00		NIST Webbook
tb	445.00	K	KDB
tb	428.00 ± 3.00	K	NIST Webbook
tb	426.55 ± 0.70	K	NIST Webbook
tb	440.65 ± 5.00	K	NIST Webbook
tc	621.20 ± 0.30	K	NIST Webbook
tc	621.20 ± 0.50	K	NIST Webbook
tc	621.20	K	KDB
tf	181.90	K	KDB
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.45	J/mol×K	639.93	Joback Method
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
dvisc	0.0001609	Pa×s	473.74	Joback Method
dvisc	0.3001577	Pa×s	210.74	Joback Method
dvisc	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.0055777	Pa×s	298.41	Joback Method
dvisc	0.0016351	Pa×s	342.24	Joback Method
dvisc	0.0006333	Pa×s	386.07	Joback Method
dvisc	0.0002977	Pa×s	429.91	Joback Method
hvapt	46.50	kJ/mol	378.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64813e+01
Coeff. B	-4.53320e+03
Coeff. C	-4.44190e+01
Temperature range (K), min.	324.36
Temperature range (K), max.	450.26

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18720655&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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=844

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume