4-Heptanol, 2-methyl-

Other names:	2-Methyl-4-heptanol
	2-Methylheptanol-(4)
	2-methylheptan-4-ol
	6-Methyl-4-heptanol
Inchi:	InChI=1S/C8H18O/c1-4-5-8(9)6-7(2)3/h7-9H,4-6H2,1-3H3
InchiKey:	QXPLZEKPCGUWEM-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCC(O)CC(C)C
Mol. weight [g/mol]:	130.23
CAS:	21570-35-4

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
tb	439.45 ± 1.00	K	NIST Webbook
tb	433.15 ± 3.00	K	NIST Webbook
tb	433.65 ± 5.00	K	NIST Webbook
tc	639.93	K	Joback Method
tf	210.74	K	Joback Method
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	346.54	J/mol×K	612.23	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
cpl	331.80	J/mol×K	298.50	NIST Webbook
dvisc	0.0001609	Pa×s	473.74	Joback Method
dvisc	0.0002977	Pa×s	429.91	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
hvapt	56.30	kJ/mol	391.00	NIST Webbook
hvapt	54.80	kJ/mol	394.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57908e+01
Coeff. B	-4.06535e+03
Coeff. C	-7.55780e+01
Temperature range (K), min.	337.80
Temperature range (K), max.	463.52

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21570354&Units=SI

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