1-Heptanol, 4-methyl-

Other names: 4-Methyl-1-heptanol
Inchi: InChI=1S/C8H18O/c1-3-5-8(2)6-4-7-9/h8-9H,3-7H2,1-2H3
InchiKey: LLUQZGDMUIMPTC-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCCC(C)CCCO
Mol. weight [g/mol]: 130.23
CAS: 817-91-4

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
mcvol	129.450	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
ripol	1973.00		NIST Webbook
tb	455.85 ± 0.50	K	NIST Webbook
tb	463.65 ± 5.00	K	NIST Webbook
tb	455.15 ± 3.00	K	NIST Webbook
tc	637.10	K	Joback Method
tf	225.74	K	Joback Method
vc	0.496	m3/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	0.0169844	Pa×s	267.15	Joback Method
dvisc	0.1178389	Pa×s	225.74	Joback Method
dvisc	0.0041171	Pa×s	308.55	Joback Method
dvisc	0.0013956	Pa×s	349.96	Joback Method
dvisc	0.0005948	Pa×s	391.37	Joback Method
dvisc	0.0002984	Pa×s	432.77	Joback Method
dvisc	0.0001689	Pa×s	474.18	Joback Method
hvapt	55.90	kJ/mol	406.50	NIST Webbook
hvapt	56.70	kJ/mol	405.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70449e+01
Coeff. B	-5.29832e+03
Coeff. C	-2.94790e+01
Temperature range (K), min.	345.66
Temperature range (K), max.	481.04

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=C817914&Units=SI

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