

2-Heptanol, 4-methyl-

Other names:	4-Methyl-2-heptanol
Inchi:	InChI=1S/C8H18O/c1-4-5-7(2)6-8(3)9/h7-9H,4-6H2,1-3H3
InchiKey:	GUHWHNUGIGOSCN-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCC(C)CC(C)O
Mol. weight [g/mol]:	130.23
CAS:	56298-90-9

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
ripol	1369.00		NIST Webbook
ripol	1375.00		NIST Webbook
tb	444.85 ± 0.50	K	NIST Webbook
tb	441.15 ± 3.00	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	290.39	J/mol×K	473.74	Joback Method
cpg	356.45	J/mol×K	639.93	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method

cpg	314.22	J/mol×K	529.14	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method
cpl	312.50	J/mol×K	298.50	NIST Webbook
dvisc	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.0001609	Pa×s	473.74	Joback Method
dvisc	0.0002977	Pa×s	429.91	Joback Method
dvisc	0.0006333	Pa×s	386.07	Joback Method
dvisc	0.0016351	Pa×s	342.24	Joback Method
dvisc	0.0055777	Pa×s	298.41	Joback Method
dvisc	0.3001577	Pa×s	210.74	Joback Method
hvapt	54.20	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61924e+01
Coeff. B	-4.47474e+03
Coeff. C	-5.82320e+01
Temperature range (K), min.	339.58
Temperature range (K), max.	469.48

Sources

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=C56298909&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/ci990307I

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

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