3-Heptanol, 4-methyl-

Other names:	4-METHYL-3-HEPTANOL
	4-METHYL-5-HEPTANOL
	4-methylheptan-3-ol
Inchi:	InChI=1S/C8H18O/c1-4-6-7(3)8(9)5-2/h7-9H,4-6H2,1-3H3
InchiKey:	BKQICAFAUMRYLZ-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCC(C)C(O)CC
Mol. weight [g/mol]:	130.23
CAS:	14979-39-6

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	428.15 ± 5.00	K	NIST Webbook
tb	428.55 ± 0.70	K	NIST Webbook
tb	443.00	K	KDB
tc	623.50 ± 0.50	K	NIST Webbook
tc	623.50	K	KDB
tc	623.50 ± 0.50	K	NIST Webbook
tf	150.00	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	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
cpg	290.39	J/mol×K	473.74	Joback Method
cpl	309.20	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	0.0006333	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	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.3001577	Pa×s	210.74	Joback Method
hvapt	43.90	kJ/mol	379.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.70	K	10.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.78515e+01
Coeff. B	-5.87879e+03
Coeff. C	1.60980e+01
Temperature range (K), min.	318.61
Temperature range (K), max.	452.71

Sources

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=843
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14979396&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume