

3-Hexanol, 3,5-dimethyl-, (.+/-.)-

Inchi:	InChI=1S/C8H18O/c1-5-8(4,9)6-7(2)3/h7,9H,5-6H2,1-4H3
InchiKey:	INMGJWCKWKKMPN-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(C)(O)CC(C)C
Mol. weight [g/mol]:	130.23
CAS:	19113-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-374.71	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	470.95	K	Joback Method
tc	643.32	K	Joback Method
tf	228.16	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.99	J/mol×K	470.95	Joback Method
cpg	305.85	J/mol×K	499.68	Joback Method
cpg	318.10	J/mol×K	528.41	Joback Method
cpg	329.77	J/mol×K	557.13	Joback Method
cpg	340.87	J/mol×K	585.86	Joback Method
cpg	351.43	J/mol×K	614.59	Joback Method
cpg	361.48	J/mol×K	643.32	Joback Method
dvisc	0.1736472	Pa×s	228.16	Joback Method
dvisc	0.0230030	Pa×s	268.62	Joback Method

dvisc	0.0051732	Pa×s	309.09	Joback Method
dvisc	0.0016435	Pa×s	349.55	Joback Method
dvisc	0.0006624	Pa×s	390.02	Joback Method
dvisc	0.0003167	Pa×s	430.49	Joback Method
dvisc	0.0001719	Pa×s	470.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	2.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19113781&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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