

DL-2-hexanol

Inchi:	InChI=1S/C6H14O/c1-3-4-5-6(2)7/h6-7H,3-5H2,1-2H3
InchiKey:	QNVRIHYSUZMSGM-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCCC(C)O
Mol. weight [g/mol]:	102.17
CAS:	20281-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-324.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.557		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	411.65 ± 3.00	K	NIST Webbook
tc	592.97	K	Joback Method
tf	203.20	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	261.25	J/mol×K	592.97	Joback Method
dvisc	0.0002400	Pa×s	428.42	Joback Method
dvisc	0.0004330	Pa×s	390.88	Joback Method

dvisc	0.0008856	Pa×s	353.35	Joback Method
dvisc	0.0021472	Pa×s	315.81	Joback Method
dvisc	0.0066108	Pa×s	278.27	Joback Method
dvisc	0.0289027	Pa×s	240.74	Joback Method
dvisc	0.2179366	Pa×s	203.20	Joback Method

Sources

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=C20281861&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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