

hexanol-d3

Inchi:	InChI=1S/C6H14O/c1-2-3-4-5-6-7/h7H,2-6H2,1H3/i1D3
InchiKey:	ZSIAUFGUXNUGDI-FIBGUPNXSA-N
Formula:	C6H11D3O
SMILES:	CCCCCO
Mol. weight [g/mol]:	105.19

Physical Properties

Property code	Value	Unit	Source
gf	-137.18	kJ/mol	Joback Method
hf	-319.40	kJ/mol	Joback Method
hfus	15.38	kJ/mol	Joback Method
hvap	45.63	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.559		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
ripol	1355.00		NIST Webbook
tb	428.86	K	Joback Method
tc	589.96	K	Joback Method
tf	218.20	K	Joback Method
vc	0.391	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.67	J/molxK	428.86	Joback Method
cpg	217.18	J/molxK	455.71	Joback Method
cpg	226.36	J/molxK	482.56	Joback Method
cpg	235.20	J/molxK	509.41	Joback Method
cpg	243.71	J/molxK	536.26	Joback Method
cpg	251.90	J/molxK	563.11	Joback Method
cpg	259.79	J/molxK	589.96	Joback Method
dvisc	0.0859852	Paxs	218.20	Joback Method
dvisc	0.0165401	Paxs	253.31	Joback Method

dvisc	0.0047527	Paxs	288.42	Joback Method
dvisc	0.0017902	Paxs	323.53	Joback Method
dvisc	0.0008164	Paxs	358.64	Joback Method
dvisc	0.0004282	Paxs	393.75	Joback Method
dvisc	0.0002497	Paxs	428.86	Joback Method

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=R329025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	McGowan's characteristic volume
pc:	Critical 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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