

Hexane, 1,1'-[methylenebis(oxy)]bis-

Other names:	1-[(Hexyloxy)methoxy]hexane
Inchi:	InChI=1S/C13H28O2/c1-3-5-7-9-11-14-13-15-12-10-8-6-4-2/h3-13H2,1-2H3
InchiKey:	SMBRWKSIANXXKZ-UHFFFAOYSA-N
Formula:	C13H28O2
SMILES:	CCCCCOCOCOSCCCC
Mol. weight [g/mol]:	216.36
CAS:	54815-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-151.42	kJ/mol	Joback Method
hf	-576.09	kJ/mol	Joback Method
hfus	31.80	kJ/mol	Joback Method
hvap	49.35	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	4.138		Crippen Method
mcvol	205.770	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
tb	541.68	K	Joback Method
tc	702.09	K	Joback Method
tf	280.73	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.66	J/molxK	541.68	Joback Method
cpg	531.55	J/molxK	568.42	Joback Method
cpg	547.86	J/molxK	595.15	Joback Method
cpg	563.59	J/molxK	621.89	Joback Method
cpg	578.76	J/molxK	648.62	Joback Method
cpg	593.36	J/molxK	675.36	Joback Method
cpg	607.40	J/molxK	702.09	Joback Method
dvisc	0.0027724	Paxs	280.73	Joback Method

dvisc	0.0011850	Paxs	324.22	Joback Method
dvisc	0.0006193	Paxs	367.71	Joback Method
dvisc	0.0003713	Paxs	411.20	Joback Method
dvisc	0.0002455	Paxs	454.70	Joback Method
dvisc	0.0001745	Paxs	498.19	Joback Method
dvisc	0.0001310	Paxs	541.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C54815122&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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