

2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethoxy)-ethanol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H26O5/c1-12(2)11-17-10-9-16-8-7-15-6-5-14-4-3-13/h12-13H,3-11H2,1-2H1

DCNSLUGOHIBLOR-UHFFFAOYSA-N

C12H26O5

CC(C)COCCOCCOCCOCCO

250.33

Physical Properties

Property code	Value	Unit	Source
gf	-509.10	kJ/mol	Joback Method
hf	-977.40	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	68.24	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	0.701		Crippen Method
mcvol	209.290	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1799.60		NIST Webbook
tb	655.38	K	Joback Method
tc	818.40	K	Joback Method
tf	359.74	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.77	J/mol×K	655.38	Joback Method
cpg	606.26	J/mol×K	682.55	Joback Method
cpg	620.20	J/mol×K	709.72	Joback Method
cpg	633.56	J/mol×K	736.89	Joback Method
cpg	646.34	J/mol×K	764.06	Joback Method
cpg	658.54	J/mol×K	791.23	Joback Method
cpg	670.14	J/mol×K	818.40	Joback Method
dvisc	0.0022984	Pa×s	359.74	Joback Method
dvisc	0.0006688	Pa×s	409.01	Joback Method

dvisc	0.0002538	Pa×s	458.29	Joback Method
dvisc	0.0001163	Pa×s	507.56	Joback Method
dvisc	0.0000611	Pa×s	556.83	Joback Method
dvisc	0.0000357	Pa×s	606.11	Joback Method
dvisc	0.0000226	Pa×s	655.38	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=R188453&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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