

2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethoxy)-ethyl acetate

Inchi:
InchiKey:
Formula:
SMILES:
Mol. weight [g/mol]:

InChI=1S/C14H28O6/c1-13(2)12-19-9-8-17-5-4-16-6-7-18-10-11-20-14(3)15/h13H,4-12H
FKJHILTXCNSWLH-UHFFFAOYSA-N
C14H28O6
CC(=O)OCCOCCOCCOCCOCC(C)C
292.37

Physical Properties

Property code	Value	Unit	Source
gf	-589.36	kJ/mol	Joback Method
hf	-1111.25	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	65.17	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	1.272		Crippen Method
mcvol	239.040	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinpol	1935.50		NIST Webbook
rinpol	1935.50		NIST Webbook
tb	685.25	K	Joback Method
tc	857.14	K	Joback Method
tf	393.62	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.89	J/mol×K	685.25	Joback Method
cpg	702.32	J/mol×K	713.90	Joback Method
cpg	718.03	J/mol×K	742.55	Joback Method
cpg	732.99	J/mol×K	771.19	Joback Method
cpg	747.19	J/mol×K	799.84	Joback Method
cpg	760.61	J/mol×K	828.49	Joback Method
cpg	773.24	J/mol×K	857.14	Joback Method
dvisc	0.0007810	Pa×s	393.62	Joback Method

dvisc	0.0003861	Pa×s	442.23	Joback Method
dvisc	0.0002194	Pa×s	490.83	Joback Method
dvisc	0.0001381	Pa×s	539.43	Joback Method
dvisc	0.0000938	Pa×s	588.04	Joback Method
dvisc	0.0000676	Pa×s	636.64	Joback Method
dvisc	0.0000510	Pa×s	685.25	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=R188468&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
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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