

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

Inchi:	InChI=1S/C12H24O5/c1-11(2)10-16-7-6-14-4-5-15-8-9-17-12(3)13/h11H,4-10H2,1-3H3
InchiKey:	ABYFRGIVTBPFIJ-UHFFFAOYSA-N
Formula:	C12H24O5
SMILES:	CC(=O)OCCOCCOCCOCC(C)C
Mol. weight [g/mol]:	248.32

Physical Properties

Property code	Value	Unit	Source
gf	-501.20	kJ/mol	Joback Method
hf	-937.75	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	1.255		Crippen Method
mvol	204.990	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1645.70		NIST Webbook
tb	617.07	K	Joback Method
tc	788.99	K	Joback Method
tf	348.85	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.50	J/molxK	617.07	Joback Method
cpg	619.67	J/molxK	760.34	Joback Method
cpg	606.67	J/molxK	731.69	Joback Method
cpg	593.03	J/molxK	703.03	Joback Method
cpg	578.79	J/molxK	674.38	Joback Method
cpg	563.94	J/molxK	645.72	Joback Method
cpg	632.03	J/molxK	788.99	Joback Method
dvisc	0.0000862	Paxs	617.07	Joback Method
dvisc	0.0001141	Paxs	572.37	Joback Method

dvisc	0.0001583	Paxs	527.66	Joback Method
dvisc	0.0002334	Paxs	482.96	Joback Method
dvisc	0.0003725	Paxs	438.26	Joback Method
dvisc	0.0006609	Paxs	393.55	Joback Method
dvisc	0.0013585	Paxs	348.85	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=R188493&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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