

2-(2-(2-Isopentoxy-ethoxy)-ethoxy)-ethoxy)-ethyl acetate

InChI: InChI=1S/C15H30O6/c1-14(2)4-5-17-6-7-18-8-9-19-10-11-20-12-13-21-15(3)16/h14H,4-
InChIKey: UDDKCGTYJUTLEO-UHFFFAOYSA-N

Formula: C15H30O6

SMILES: CC(=O)OCCOCCOCCOCCOCCC(C)C

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-580.94	kJ/mol	Joback Method
hf	-1131.89	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.662		Crippen Method
mcvol	253.130	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinsol	2034.80		NIST Webbook
tb	708.13	K	Joback Method
tc	880.67	K	Joback Method
tf	404.89	K	Joback Method
vc	0.966	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.38	J/molxK	708.13	Joback Method
cpg	759.30	J/molxK	736.89	Joback Method
cpg	775.43	J/molxK	765.64	Joback Method
cpg	790.75	J/molxK	794.40	Joback Method
cpg	805.24	J/molxK	823.16	Joback Method
cpg	818.89	J/molxK	851.91	Joback Method
cpg	831.69	J/molxK	880.67	Joback Method
dvisc	0.0007081	Paxs	404.89	Joback Method
dvisc	0.0003456	Paxs	455.43	Joback Method

dvisc	0.0001947	Paxs	505.97	Joback Method
dvisc	0.0001217	Paxs	556.51	Joback Method
dvisc	0.0000823	Paxs	607.05	Joback Method
dvisc	0.0000591	Paxs	657.59	Joback Method
dvisc	0.0000445	Paxs	708.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188542&Units=SI
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

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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