

1-[(1-Propoxypropan-2-yl)oxy]propan-2-yl acetate

Inchi:	InChI=1S/C11H22O4/c1-5-6-13-7-9(2)14-8-10(3)15-11(4)12/h9-10H,5-8H2,1-4H3
InchiKey:	PNBCGVPSRHMZDO-UHFFFAOYSA-N
Formula:	C11H22O4
SMILES:	CCCOCC(C)OCC(C)OC(C)=O
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	-407.06	kJ/mol	Joback Method
hf	-790.17	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	53.28	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.770		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1312.00		NIST Webbook
tb	571.33	K	Joback Method
tc	747.59	K	Joback Method
tf	300.35	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.00	J/mol×K	571.33	Joback Method
cpg	485.22	J/mol×K	600.71	Joback Method
cpg	499.87	J/mol×K	630.08	Joback Method
cpg	513.94	J/mol×K	659.46	Joback Method
cpg	527.44	J/mol×K	688.84	Joback Method
cpg	540.34	J/mol×K	718.21	Joback Method
cpg	552.64	J/mol×K	747.59	Joback Method
dvisc	0.0028826	Pa×s	300.35	Joback Method

dvisc	0.0011893	Pa×s	345.51	Joback Method
dvisc	0.0006021	Pa×s	390.68	Joback Method
dvisc	0.0003510	Pa×s	435.84	Joback Method
dvisc	0.0002265	Pa×s	481.00	Joback Method
dvisc	0.0001575	Pa×s	526.17	Joback Method
dvisc	0.0001160	Pa×s	571.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378331&Units=SI
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

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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