

2-(2-Pentoxyethoxy)ethyl acetate

Other names:	Diethylene glycol, pentyl ether, acetate
Inchi:	InChI=1S/C11H22O4/c1-3-4-5-6-13-7-8-14-9-10-15-11(2)12/h3-10H2,1-2H3
InchiKey:	MSHVPEDOYHYTBV-UHFFFAOYSA-N
Formula:	C11H22O4
SMILES:	CCCCCOCCOCCOC(C)=O
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	-402.18	kJ/mol	Joback Method
hf	-779.61	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.773		Crippen Method
mvol	185.030	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1507.00		NIST Webbook
tb	572.21	K	Joback Method
tc	742.45	K	Joback Method
tf	330.35	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.34	J/molxK	572.21	Joback Method
cpg	483.93	J/molxK	600.58	Joback Method
cpg	498.01	J/molxK	628.96	Joback Method
cpg	511.57	J/molxK	657.33	Joback Method
cpg	524.60	J/molxK	685.70	Joback Method
cpg	537.09	J/molxK	714.07	Joback Method
cpg	549.04	J/molxK	742.45	Joback Method
dvisc	0.0016203	Paxs	330.35	Joback Method

dvisc	0.0008503	Paxs	370.66	Joback Method
dvisc	0.0005064	Paxs	410.97	Joback Method
dvisc	0.0003308	Paxs	451.28	Joback Method
dvisc	0.0002318	Paxs	491.59	Joback Method
dvisc	0.0001714	Paxs	531.90	Joback Method
dvisc	0.0001322	Paxs	572.21	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=R188780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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