

Ethylene glycol, O-acetyl-, O'-(2-acetyloxy)benzoate

Inchi:	InChI=1S/C13H14O6/c1-9(14)17-7-8-18-13(16)11-5-3-4-6-12(11)19-10(2)15/h3-6H,7-8H
InchiKey:	LCTKGQSNPMBONU-UHFFFAOYSA-N
Formula:	C13H14O6
SMILES:	CC(=O)OCCOC(=O)c1ccccc1OC(C)=O
Mol. weight [g/mol]:	266.25

Physical Properties

Property code	Value	Unit	Source
gf	-540.40	kJ/mol	Joback Method
hf	-820.99	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.332		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1859.00		NIST Webbook
tb	757.37	K	Joback Method
tc	970.44	K	Joback Method
tf	491.69	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.41	J/molxK	757.37	Joback Method
cpg	578.41	J/molxK	934.93	Joback Method
cpg	570.13	J/molxK	899.42	Joback Method
cpg	560.88	J/molxK	863.91	Joback Method
cpg	550.67	J/molxK	828.39	Joback Method
cpg	539.51	J/molxK	792.88	Joback Method
cpg	585.70	J/molxK	970.44	Joback Method
dvisc	0.0001026	Paxs	757.37	Joback Method
dvisc	0.0001273	Paxs	713.09	Joback Method

dvisc	0.0001623	Paxs	668.81	Joback Method
dvisc	0.0002143	Paxs	624.53	Joback Method
dvisc	0.0002953	Paxs	580.25	Joback Method
dvisc	0.0004289	Paxs	535.97	Joback Method
dvisc	0.0006662	Paxs	491.69	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=U374700&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

Latest version available from:

<https://www.chemeo.com/cid/65-429-4/Ethylene-glycol-O-acetyl-O-2-acetyloxy-benzoate.pdf>

Generated by Cheméo on 2024-04-19 22:08:14.490670305 +0000 UTC m=+15853743.411247616.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.