Acetic acid 4,5-diethoxy-2-ethoxymethyl-tetrahydro-pyran-3-y ester

Inchi: InChI=1S/C14H26O6/c1-5-16-8-11-14(20-10(4)15)13(18-7-3)12(9-19-11)17-6-2/h11-14H

InchiKey: HASLUHNTFKIGQN-UHFFFAOYSA-N

Formula: C14H26O6

SMILES: CCOCC1OCC(OCC)C(OCC)C1OC(C)=O

Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-566.72	kJ/mol	Joback Method
hf	-1112.45	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.164		Crippen Method
mcvol	228.180	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1674.13		NIST Webbook
rinpol	1690.13		NIST Webbook
rinpol	1693.85		NIST Webbook
tb	695.76	K	Joback Method
tc	885.66	K	Joback Method
tf	407.62	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.38	J/mol×K	695.76	Joback Method
cpg	776.35	J/mol×K	854.01	Joback Method
cpg	761.55	J/mol×K	822.36	Joback Method
cpg	745.62	J/mol×K	790.71	Joback Method
cpg	728.59	J/mol×K	759.06	Joback Method
cpg	710.50	J/mol×K	727.41	Joback Method
cpg	789.99	J/mol×K	885.66	Joback Method

dvisc	0.0001221	Pa×s	695.76	Joback Method
dvisc	0.0001507	Pa×s	647.74	Joback Method
dvisc	0.0001922	Pa×s	599.71	Joback Method
dvisc	0.0002559	Pa×s	551.69	Joback Method
dvisc	0.0003598	Pa×s	503.67	Joback Method
dvisc	0.0005435	Pa×s	455.64	Joback Method
dvisc	0.0009048	Pa×s	407.62	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=R262472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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