Acetic acid 5-ethoxy-2-ethoxymethyl-4-methoxy-tetrahydro-p ester

Inchi: InChI=1S/C13H24O6/c1-5-16-7-10-13(19-9(3)14)12(15-4)11(8-18-10)17-6-2/h10-13H,5-8
InchiKey: XOVGGTUZRVHREC-UHFFFAOYSA-N
Formula: C13H24O6
SMILES: CCOCC1OCC(OCC)C(OC)C1OC(C)=O
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-575.14	kJ/mol	Joback Method
hf	-1091.81	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.774		Crippen Method
mcvol	214.090	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1652.98		NIST Webbook
rinpol	1648.21		NIST Webbook
rinpol	1631.63		NIST Webbook
rinpol	1631.63		NIST Webbook
tb	672.88	K	Joback Method
tc	864.28	K	Joback Method
tf	396.35	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.91	J/mol×K	672.88	Joback Method
cpg	653.74	J/mol×K	704.78	Joback Method
cpg	671.60	J/mol×K	736.68	Joback Method
cpg	688.45	J/mol×K	768.58	Joback Method
cpg	704.27	J/mol×K	800.48	Joback Method
cpg	719.02	J/mol×K	832.38	Joback Method

cpg	732.66	J/mol×K	864.28	Joback Method
dvisc	0.0009507	Pa×s	396.35	Joback Method
dvisc	0.0005805	Pa×s	442.44	Joback Method
dvisc	0.0003890	Pa×s	488.53	Joback Method
dvisc	0.0002793	Pa×s	534.62	Joback Method
dvisc	0.0002114	Pa×s	580.70	Joback Method
dvisc	0.0001667	Pa×s	626.79	Joback Method
dvisc	0.0001357	Pa×s	672.88	Joback Method

Sources

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=R262521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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