

Acetic acid

5-ethoxy-4-methoxy-2-methoxymethyl-tetrahydro-

InChI:
ester

InChI=1S/C12H22O6/c1-5-16-10-7-17-9(6-14-3)12(11(10)15-4)18-8(2)13/h9-12H,5-7H2,

InChIKey:

JHTBHOSCGRZUIW-UHFFFAOYSA-N

Formula:

C12H22O6

SMILES:

CCOC1COC(COC)C(OC(C)=O)C1OC

Mol. weight [g/mol]:

262.30

Physical Properties

Property code	Value	Unit	Source
gf	-583.56	kJ/mol	Joback Method
hf	-1071.17	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	62.70	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.383		Crippen Method
mcvol	200.000	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1571.51		NIST Webbook
rinpol	1586.92		NIST Webbook
rinpol	1595.61		NIST Webbook
rinpol	1571.51		NIST Webbook
tb	650.00	K	Joback Method
tc	843.28	K	Joback Method
tf	385.08	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.70	J/molxK	650.00	Joback Method
cpg	598.16	J/molxK	682.21	Joback Method
cpg	615.71	J/molxK	714.43	Joback Method
cpg	632.32	J/molxK	746.64	Joback Method
cpg	647.96	J/molxK	778.86	Joback Method
cpg	662.58	J/molxK	811.07	Joback Method

cpg	676.15	J/mol×K	843.28	Joback Method
dvisc	0.0009905	Paxs	385.08	Joback Method
dvisc	0.0006152	Paxs	429.23	Joback Method
dvisc	0.0004176	Paxs	473.39	Joback Method
dvisc	0.0003028	Paxs	517.54	Joback Method
dvisc	0.0002310	Paxs	561.69	Joback Method
dvisc	0.0001833	Paxs	605.85	Joback Method
dvisc	0.0001501	Paxs	650.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R262536&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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