Ethyl hematommate

Inchi: InChI=1S/C11H12O5/c1-3-16-11(15)9-6(2)4-8(13)7(5-12)10(9)14/h4-5,13-14H,3H2,1-2H
InchiKey: HUXJGSHUVDWZAM-UHFFFAOYSA-N
Formula: C11H12O5
SMILES: CCOC(=O)c1c(C)cc(O)c(C=O)c1O
Mol. weight [g/mol]: 224.21
CAS: 39503-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-507.79	kJ/mol	Joback Method
hf	-741.78	kJ/mol	Joback Method
hfus	34.15	kJ/mol	Joback Method
hvap	85.58	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.395		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1765.10		NIST Webbook
tb	773.91	K	Joback Method
tc	1004.32	K	Joback Method
tf	602.79	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.83	J/mol×K	773.91	Joback Method
cpg	460.69	J/mol×K	812.31	Joback Method
cpg	470.18	J/mol×K	850.71	Joback Method
cpg	479.39	J/mol×K	889.11	Joback Method
cpg	488.43	J/mol×K	927.52	Joback Method
cpg	497.39	J/mol×K	965.92	Joback Method
cpg	506.38	J/mol×K	1004.32	Joback Method
dvisc	0.0000129	Pa×s	602.79	Joback Method

dvisc	0.0000077	Pa×s	631.31	Joback Method
dvisc	0.0000048	Pa×s	659.83	Joback Method
dvisc	0.0000031	Pa×s	688.35	Joback Method
dvisc	0.0000021	Pa×s	716.87	Joback Method
dvisc	0.0000015	Pa×s	745.39	Joback Method
dvisc	0.0000010	Pa×s	773.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C39503145&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