

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.83	J/molxK	773.91	Joback Method
cpg	497.39	J/molxK	965.92	Joback Method
cpg	488.43	J/molxK	927.52	Joback Method
cpg	479.39	J/molxK	889.11	Joback Method
cpg	470.18	J/molxK	850.71	Joback Method
cpg	460.69	J/molxK	812.31	Joback Method
cpg	506.38	J/molxK	1004.32	Joback Method
dvisc	0.0000010	Paxs	773.91	Joback Method

dvisc	0.0000015	Paxs	745.39	Joback Method
dvisc	0.0000021	Paxs	716.87	Joback Method
dvisc	0.0000031	Paxs	688.35	Joback Method
dvisc	0.0000048	Paxs	659.83	Joback Method
dvisc	0.0000077	Paxs	631.31	Joback Method
dvisc	0.0000129	Paxs	602.79	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=C39503145&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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