MEXILETINE, M (DESAMINO-OXO-HO-) ISOMER 3, AC

Inchi: InChI=1S/C13H16O4/c1-8-5-12(17-11(4)15)6-9(2)13(8)16-7-10(3)14/h5-6H,7H2,1-4H3
InchiKey: KEZJMWTUAZTVQH-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: CC(=O)COc1c(C)cc(OC(C)=O)cc1C
Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
gf	-325.74	kJ/mol	Joback Method
hf	-599.13	kJ/mol	Joback Method
hfus	27.87	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.197		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	691.04	K	Joback Method
tc	901.40	K	Joback Method
tf	444.57	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.63	J/mol×K	691.04	Joback Method
cpg	499.26	J/mol×K	726.10	Joback Method
cpg	512.08	J/mol×K	761.16	Joback Method
cpg	524.10	J/mol×K	796.22	Joback Method
cpg	535.29	J/mol×K	831.28	Joback Method
cpg	545.65	J/mol×K	866.34	Joback Method
cpg	555.18	J/mol×K	901.40	Joback Method
dvisc	0.0007449	Pa×s	444.57	Joback Method

dvisc	0.0004947	Pa×s	485.65	Joback Method
dvisc	0.0003503	Pa×s	526.73	Joback Method
dvisc	0.0002607	Pa×s	567.81	Joback Method
dvisc	0.0002019	Pa×s	608.88	Joback Method
dvisc	0.0001615	Pa×s	649.96	Joback Method
dvisc	0.0001327	Pa×s	691.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255271&Units=SI
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

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