

MEXILETINE, M(DESAMINO-OXO-HO-)ISOMER 1, 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	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	691.04	K	Joback Method
tc	901.40	K	Joback Method
tf	444.57	K	Joback Method
vc	0.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.63	J/molxK	691.04	Joback Method
cpg	545.65	J/molxK	866.34	Joback Method
cpg	535.29	J/molxK	831.28	Joback Method
cpg	524.10	J/molxK	796.22	Joback Method
cpg	512.08	J/molxK	761.16	Joback Method
cpg	499.26	J/molxK	726.10	Joback Method
cpg	555.18	J/molxK	901.40	Joback Method
dvisc	0.0001327	Paxs	691.04	Joback Method

dvisc	0.0001615	Paxs	649.96	Joback Method
dvisc	0.0002019	Paxs	608.88	Joback Method
dvisc	0.0002607	Paxs	567.81	Joback Method
dvisc	0.0003503	Paxs	526.73	Joback Method
dvisc	0.0004947	Paxs	485.65	Joback Method
dvisc	0.0007449	Paxs	444.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255251&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

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