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

Inchi: InChI=1S/C15H20O5/c1-9-6-14(20-13(5)17)7-10(2)15(9)18-8-11(3)19-12(4)16/h6-7,11H,

InchiKey: CSZXIHIQDZFRQA-UHFFFAOYSA-N

Formula: C15H20O5

SMILES: CC(=O)Oc1cc(C)c(OCC(C)OC(C)=O)c(C)c1

Mol. weight [g/mol]: 280.32

Physical Properties

Property code	Value	Unit	Source
gf	-416.34	kJ/mol	Joback Method
hf	-777.91	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.559		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	758.78	K	Joback Method
tc	965.88	K	Joback Method
tf	474.34	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.61	J/mol×K	758.78	Joback Method
cpg	634.06	J/mol×K	793.30	Joback Method
cpg	647.53	J/mol×K	827.81	Joback Method
cpg	660.02	J/mol×K	862.33	Joback Method
cpg	671.49	J/mol×K	896.85	Joback Method
cpg	681.94	J/mol×K	931.36	Joback Method
cpg	691.36	J/mol×K	965.88	Joback Method
dvisc	0.0005428	Pa×s	474.34	Joback Method

dvisc	0.0003363	Pa×s	521.75	Joback Method
dvisc	0.0002257	Pa×s	569.15	Joback Method
dvisc	0.0001610	Pa×s	616.56	Joback Method
dvisc	0.0001206	Pa×s	663.97	Joback Method
dvisc	0.0000938	Pa×s	711.37	Joback Method
dvisc	0.0000753	Pa×s	758.78	Joback Method

Sources

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=R255211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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