

MEXILETINE, M(DESAMINO-DI-HO) ISOMER 2, 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:	CSZXIHQDZFRQA-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	1930.00		NIST Webbook
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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/molxK	758.78	Joback Method
cpg	681.94	J/molxK	931.36	Joback Method
cpg	671.49	J/molxK	896.85	Joback Method
cpg	660.02	J/molxK	862.33	Joback Method
cpg	647.53	J/molxK	827.81	Joback Method
cpg	634.06	J/molxK	793.30	Joback Method
cpg	691.36	J/molxK	965.88	Joback Method
dvisc	0.0000753	Paxs	758.78	Joback Method

dvisc	0.0000938	Paxs	711.37	Joback Method
dvisc	0.0001206	Paxs	663.97	Joback Method
dvisc	0.0001610	Paxs	616.56	Joback Method
dvisc	0.0002257	Paxs	569.15	Joback Method
dvisc	0.0003363	Paxs	521.75	Joback Method
dvisc	0.0005428	Paxs	474.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255226&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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