TOCAINIDE, M(HO-), AC

Inchi: InChI=1S/C15H20N2O4/c1-8-6-13(21-12(5)19)7-9(2)14(8)17-15(20)10(3)16-11(4)18/h6-1
InchiKey: ULHFVVKKZLEKQA-UHFFFAOYSA-N
Formula: C15H20N2O4
SMILES: CC(=O)NC(C)C(=O)Nc1c(C)cc(OC(C)=O)cc1C
Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-156.48	kJ/mol	Joback Method
hf	-519.11	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	88.38	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	1.692		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	868.15	K	Joback Method
tc	1086.10	K	Joback Method
tf	585.13	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.75	J/mol×K	868.15	Joback Method
cpg	698.79	J/mol×K	904.47	Joback Method
cpg	709.76	J/mol×K	940.80	Joback Method
cpg	719.69	J/mol×K	977.12	Joback Method
cpg	728.60	J/mol×K	1013.45	Joback Method
cpg	736.49	J/mol×K	1049.77	Joback Method
cpg	743.39	J/mol×K	1086.10	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=R255459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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