TOCAINIDE, AC

Inchi: InChI=1S/C13H18N2O2/c1-8-6-5-7-9(2)12(8)15-13(17)10(3)14-11(4)16/h5-7,10H,1-4H3,
InchiKey: GEHWZSUZEPBZNQ-UHFFFAOYSA-N
Formula: C13H18N2O2
SMILES: CC(=O)NC(C)C(=O)Nc1c(C)cccc1C
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	70.23	kJ/mol	Joback Method
hf	-221.56	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.767		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	741.12	K	Joback Method
tc	957.67	K	Joback Method
tf	477.91	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.74	J/mol×K	741.12	Joback Method
cpg	553.33	J/mol×K	777.21	Joback Method
cpg	565.98	J/mol×K	813.30	Joback Method
cpg	577.73	J/mol×K	849.40	Joback Method
cpg	588.61	J/mol×K	885.49	Joback Method
cpg	598.65	J/mol×K	921.58	Joback Method
cpg	607.89	J/mol×K	957.67	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=R255444&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