IONONE

Other names: Iraldeine
Irisone
Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6-8,12H,5,9H2,1-4H3/b8-7-
InchiKey: UZFLPKAIBPNNCA-BQYQJAHWSA-N
Formula: C13H20O
SMILES: CC(=O)/C=C/C1C(C)=CCCC1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	18.67	kJ/mol	Joback Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1423.60		NIST Webbook
rinpol	1423.60		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1424.30		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1433.00		NIST Webbook
ripol	1842.30		NIST Webbook
ripol	1846.20		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.46	J/mol×K	574.13	Joback Method
cpg	457.12	J/mol×K	610.47	Joback Method
cpg	474.66	J/mol×K	646.81	Joback Method
cpg	491.22	J/mol×K	683.15	Joback Method
cpg	506.92	J/mol×K	719.49	Joback Method
cpg	521.90	J/mol×K	755.83	Joback Method
cpg	536.27	J/mol×K	792.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C8013909&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices