

Cyperotundone

Inchi:	InChI=1S/C15H22O/c1-9-5-6-11-7-12-10(2)13(16)8-15(9,12)14(11,3)4/h9,11H,5-8H2,1-4
InchiKey:	GIGKXOAUYMWORB-CCUNJIBTSA-N
Formula:	C15H22O
SMILES:	CC1=C2CC3CCC(C)C2(CC1=O)C3(C)C
Mol. weight [g/mol]:	218.33
CAS:	3466-15-7

Physical Properties

Property code	Value	Unit	Source
gf	102.89	kJ/mol	Joback Method
hf	-239.57	kJ/mol	Joback Method
hfus	13.24	kJ/mol	Joback Method
hvap	52.32	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1717.60		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	644.11	K	Joback Method
tc	883.54	K	Joback Method
tf	443.17	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.11	J/molxK	644.11	Joback Method
cpg	562.10	J/molxK	684.01	Joback Method
cpg	582.11	J/molxK	723.92	Joback Method

cpg	601.45	J/mol×K	763.82	Joback Method
cpg	620.44	J/mol×K	803.73	Joback Method
cpg	639.37	J/mol×K	843.63	Joback Method
cpg	658.57	J/mol×K	883.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3466157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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