

Cyperotundone

Inchi:

InChI=1S/C15H22O/c1-9-11-7-10-5-6-15(4,14(10,2)3)12(11)8-13(9)16/h10,12H,5-8H2,1-

InchiKey:

UUXICWBSFZDYLB-PJRDJYAKSA-N

Formula:

C15H22O

SMILES:

CC1=C2CC3CCC(C)(C2CC1=O)C3(C)C

Mol. weight [g/mol]:

218.33

Physical Properties

Property code	Value	Unit	Source
hf	-162.15	kJ/mol	Cheméo Relay (1.0)
hfus	13.24	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	549.65	K	Cheméo Relay (1.0)
tf	474.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.11	J/mol×K	644.11	Joback Method
cpg	562.10	J/mol×K	684.01	Joback Method
cpg	582.11	J/mol×K	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=R258849&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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