

Cyperol

Inchi:

InChI=1S/C15H24O/c1-10(2)12-5-7-15(4)8-6-14(16)11(3)13(15)9-12/h12,14,16H,1,5-9H2

InchiKey:

APWLDLGOYJHNIK-AEGPPILISA-N

Formula:

C15H24O

SMILES:

C=C(C)C1CCC2(C)CCC(O)C(C)=C2C1

Mol. weight [g/mol]:

220.35

Physical Properties

Property code	Value	Unit	Source
gf	88.49	kJ/mol	Joback Method
hf	-238.82	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	666.59	K	Joback Method
tc	875.76	K	Joback Method
tf	371.17	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.00	J/mol×K	666.59	Joback Method
cpg	590.73	J/mol×K	701.45	Joback Method
cpg	608.54	J/mol×K	736.31	Joback Method
cpg	625.54	J/mol×K	771.17	Joback Method
cpg	641.88	J/mol×K	806.04	Joback Method
cpg	657.66	J/mol×K	840.90	Joback Method
cpg	673.03	J/mol×K	875.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R621039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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