7-Isopropenyl-1,4a-dimethyl-4,4a,5,6,7,8-hexahydr

Other names: «alpha»-Cyperone
Inchi: InChI=1S/C15H22O/c1-10(2)12-5-7-15(4)8-6-14(16)11(3)13(15)9-12/h12H,1,5-9H2,2-4H
InchiKey: KUFXJZXMWHNCEH-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC2(C)CCC(=O)C(C)=C2C1
Mol. weight [g/mol]: 218.33
CAS: 473-08-5

Physical Properties

Property code	Value	Unit	Source
gf	110.43	kJ/mol	Joback Method
hf	-203.95	kJ/mol	Joback Method
hfus	13.54	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1758.50		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1706.00		NIST Webbook
tb	646.90	K	Joback Method
tc	885.57	K	Joback Method
tf	382.81	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.47	J/mol×K	646.90	Joback Method
cpg	560.03	J/mol×K	686.68	Joback Method

cpg	580.39	J/mol×K	726.46	Joback Method
cpg	599.70	J/mol×K	766.24	Joback Method
cpg	618.11	J/mol×K	806.02	Joback Method
cpg	635.78	J/mol×K	845.79	Joback Method
cpg	652.86	J/mol×K	885.57	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=C473085&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