Eudesma-4,6-dien-3-one («beta»-cyperone)

Other names: Eudesma-4,6-dien-3-one
Inchi: InChI=1S/C15H22O/c1-10(2)12-5-7-15(4)8-6-14(16)11(3)13(15)9-12/h9-10H,5-8H2,1-4H
InchiKey: NUIFDRMJKLJEJE-HNNXBMFYSA-N
Formula: C15H22O
SMILES: CC1=C2C=C(C(C)C)CCC2(C)CCC1=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	56.74	kJ/mol	Joback Method
hf	-258.22	kJ/mol	Joback Method
hfus	12.37	kJ/mol	Joback Method
hvap	55.09	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	658.71	K	Joback Method
tc	896.19	K	Joback Method
tf	401.05	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.29	J/mol×K	658.71	Joback Method
cpg	557.70	J/mol×K	698.29	Joback Method
cpg	577.04	J/mol×K	737.87	Joback Method
cpg	595.44	J/mol×K	777.45	Joback Method
cpg	613.05	J/mol×K	817.03	Joback Method
cpg	630.02	J/mol×K	856.61	Joback Method

cpg	646.49	J/mol×K	896.19	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=R199101&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

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