«beta»-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

Physical Properties

Property code	Value	Unit	Source
hfus	13.54	kJ/mol	Joback Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1766.00		NIST Webbook
ripol	2403.00		NIST Webbook
ripol	2403.00		NIST Webbook

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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420212&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices