(4S,5S)-Germacrone-4,5-epoxide

Inchi: InChI=1S/C15H22O2/c1-10(2)12-9-14-15(4,17-14)7-5-6-11(3)8-13(12)16/h6,14H,5,7-9H2
InchiKey: DWGVRYKQVZGSIB-WTMFUUHESA-N
Formula: C15H22O2
SMILES: CC1=CCCC2(C)OC2CC(=C(C)C)C(=O)C1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-20.54	kJ/mol	Joback Method
hf	-380.04	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.570		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1835.00		NIST Webbook
tb	683.10	K	Joback Method
tc	927.22	K	Joback Method
tf	405.46	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.52	J/mol×K	683.10	Joback Method
cpg	596.90	J/mol×K	723.79	Joback Method
cpg	617.12	J/mol×K	764.47	Joback Method
cpg	636.33	J/mol×K	805.16	Joback Method
cpg	654.67	J/mol×K	845.85	Joback Method
cpg	672.29	J/mol×K	886.53	Joback Method
cpg	689.35	J/mol×K	927.22	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=R587667&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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