Polygodial

Inchi: InChI=1S/C15H22O2/c1-14(2)7-4-8-15(3)12(10-17)11(9-16)5-6-13(14)15/h5,9-10,12-13H
InchiKey: AZJUJOFIHHNCSV-PIMMBPRGSA-N
Formula: C15H22O2
SMILES: CC1(C)CCCC2(C)C(C=O)C(C=O)=CCC12
Mol. weight [g/mol]: 234.33
CAS: 6754-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-56.59	kJ/mol	Joback Method
hf	-367.02	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.163		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	665.76	K	Joback Method
tc	894.37	K	Joback Method
tf	417.21	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.26	J/mol×K	665.76	Joback Method
cpg	592.88	J/mol×K	703.86	Joback Method
cpg	611.61	J/mol×K	741.96	Joback Method
cpg	629.73	J/mol×K	780.06	Joback Method
cpg	647.48	J/mol×K	818.17	Joback Method
cpg	665.12	J/mol×K	856.27	Joback Method
cpg	682.89	J/mol×K	894.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6754207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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