Platambin-1,6-dione

Inchi: InChI=1S/C15H22O2/c1-9(2)11-7-8-15(4)12(16)6-5-10(3)13(15)14(11)17/h9,11,13H,3,5-
InchiKey: GNOBKKNJWOFLHO-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C1CCC(=O)C2(C)CCC(C(C)C)C(=O)C12
Mol. weight [g/mol]: 234.33
CAS: 58556-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-59.22	kJ/mol	Joback Method
hf	-433.51	kJ/mol	Joback Method
hfus	11.59	kJ/mol	Joback Method
hvap	56.30	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.163		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	703.09	K	Joback Method
tc	947.07	K	Joback Method
tf	435.39	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.39	J/mol×K	703.09	Joback Method
cpg	623.69	J/mol×K	743.75	Joback Method
cpg	644.78	J/mol×K	784.42	Joback Method
cpg	664.77	J/mol×K	825.08	Joback Method
cpg	683.75	J/mol×K	865.74	Joback Method
cpg	701.84	J/mol×K	906.40	Joback Method
cpg	719.15	J/mol×K	947.07	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=C58556835&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