Integrifolian-1,5-dione

Inchi: InChI=1S/C15H24O2/c1-10-5-6-13(17)15(4)8-11(15)7-14(2,3)9-12(10)16/h10-11H,5-9H2
InchiKey: KNPZDKSAZHSFTN-JRPNMDOOSA-N
Formula: C15H24O2
SMILES: CC1CCC(=O)C2(C)CC2CC(C)(C)CC1=O
Mol. weight [g/mol]: 236.35
CAS: 153666-26-3

Physical Properties

Property code	Value	Unit	Source
gf	-135.16	kJ/mol	Joback Method
hf	-523.73	kJ/mol	Joback Method
hfus	8.94	kJ/mol	Joback Method
hvap	55.24	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.387		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1745.00		NIST Webbook
tb	704.21	K	Joback Method
tc	958.47	K	Joback Method
tf	452.85	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.22	J/mol×K	704.21	Joback Method
cpg	652.03	J/mol×K	746.59	Joback Method
cpg	675.84	J/mol×K	788.96	Joback Method
cpg	698.88	J/mol×K	831.34	Joback Method
cpg	721.40	J/mol×K	873.72	Joback Method
cpg	743.64	J/mol×K	916.09	Joback Method
cpg	765.84	J/mol×K	958.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C153666263&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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