Faurinone

Inchi: InChI=1S/C15H26O/c1-10(2)12-7-9-15(4)8-5-6-13(15)14(12)11(3)16/h10,12-14H,5-9H2,1
InchiKey: SSCVGFQOFLDIGI-FFHGMXDLSA-N
Formula: C15H26O
SMILES: CC(=O)C1C(C(C)C)CCC2(C)CCCC12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	8.35	kJ/mol	Joback Method
hf	-369.11	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	613.22	K	Joback Method
tc	831.03	K	Joback Method
tf	334.48	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.80	J/mol×K	613.22	Joback Method
cpg	593.78	J/mol×K	649.52	Joback Method
cpg	615.41	J/mol×K	685.82	Joback Method
cpg	635.85	J/mol×K	722.13	Joback Method
cpg	655.24	J/mol×K	758.43	Joback Method
cpg	673.72	J/mol×K	794.73	Joback Method
cpg	691.44	J/mol×K	831.03	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=R224930&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