Curcumenone

Inchi: InChI=1S/C15H22O2/c1-9(2)11-7-13-12(6-5-10(3)16)15(13,4)8-14(11)17/h12-13H,5-8H2
InchiKey: HUZJLWLCLJEXEL-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC(=O)CCC1C2CC(=C(C)C)C(=O)CC12C
Mol. weight [g/mol]: 234.33
CAS: 100347-96-4

Physical Properties

Property code	Value	Unit	Source
gf	-42.98	kJ/mol	Joback Method
hf	-402.63	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.307		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1844.40		NIST Webbook
rinpol	1844.40		NIST Webbook
tb	684.13	K	Joback Method
tc	905.35	K	Joback Method
tf	425.38	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.27	J/mol×K	684.13	Joback Method
cpg	598.93	J/mol×K	721.00	Joback Method
cpg	616.72	J/mol×K	757.87	Joback Method
cpg	633.78	J/mol×K	794.74	Joback Method
cpg	650.27	J/mol×K	831.61	Joback Method
cpg	666.33	J/mol×K	868.48	Joback Method
cpg	682.11	J/mol×K	905.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100347964&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