Curcumenol

Inchi: InChI=1S/C15H22O2/c1-9(2)13-8-14-11(4)5-6-12(14)10(3)7-15(13,16)17-14/h7,11-12,16
InchiKey: ISFMXVMWEWLJGJ-DGHYUSQUSA-N
Formula: C15H22O2
SMILES: CC1=CC2(O)OC3(CC2=C(C)C)C(C)CCC13
Mol. weight [g/mol]: 234.33
CAS: 19431-84-6

Physical Properties

Property code	Value	Unit	Source
gf	49.08	kJ/mol	Joback Method
hf	-308.39	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.177		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1734.50		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1734.50		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	696.96	K	Joback Method
tc	912.86	K	Joback Method
tf	446.22	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.31	J/mol×K	696.96	Joback Method
cpg	598.15	J/mol×K	732.94	Joback Method
cpg	614.54	J/mol×K	768.93	Joback Method

cpg	630.74	J/mol×K	804.91	Joback Method
cpg	647.03	J/mol×K	840.89	Joback Method
cpg	663.66	J/mol×K	876.88	Joback Method
cpg	680.91	J/mol×K	912.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19431846&Units=SI

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