Curcumol

Inchi: InChI=1S/C15H22O2/c1-9(2)13-8-14-11(4)5-6-12(14)10(3)7-15(13,16)17-14/h11-12,16H
InchiKey: DEBDFZGNZTYPMF-YPRXJGMQSA-N
Formula: C15H22O2
SMILES: C=C1CC2(O)OC3(CC2=C(C)C)C(C)CCC13
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	81.83	kJ/mol	Joback Method
hf	-270.46	kJ/mol	Joback Method
hfus	23.21	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.177		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
ripol	2360.00		NIST Webbook
tb	691.98	K	Joback Method
tc	906.89	K	Joback Method
tf	446.62	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.01	J/mol×K	691.98	Joback Method
cpg	597.98	J/mol×K	727.80	Joback Method
cpg	614.44	J/mol×K	763.62	Joback Method
cpg	630.66	J/mol×K	799.43	Joback Method
cpg	646.90	J/mol×K	835.25	Joback Method
cpg	663.43	J/mol×K	871.07	Joback Method
cpg	680.50	J/mol×K	906.89	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=R627973&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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