

Curcumol

Inchi:	InChI=1S/C15H24O2/c1-9(2)13-8-14-11(4)5-6-12(14)10(3)7-15(13,16)17-14/h9,11-13,16
InchiKey:	QRMPRVXWPCLVNI-ARJVPZMDSA-N
Formula:	C15H24O2
SMILES:	C=C1CC2(O)OC3(CC2C(C)C)C(C)CCC13
Mol. weight [g/mol]:	236.35
CAS:	4871-97-0

Physical Properties

Property code	Value	Unit	Source
gf	34.77	kJ/mol	Joback Method
hf	-362.32	kJ/mol	Joback Method
hfus	21.74	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.112		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1594.00		NIST Webbook
ripol	2360.00		NIST Webbook
tb	680.35	K	Joback Method
tc	890.25	K	Joback Method
tf	430.98	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.74	J/molxK	680.35	Joback Method
cpg	626.04	J/molxK	715.33	Joback Method
cpg	643.67	J/molxK	750.32	Joback Method
cpg	660.86	J/molxK	785.30	Joback Method
cpg	677.84	J/molxK	820.28	Joback Method
cpg	694.87	J/molxK	855.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4871970&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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