

«alpha»-curcumene dihydro(+)

Inchi:	InChI=1S/C15H26/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h8-10,12,14-15H,5-7,11H2,
InchiKey:	XIFQPGDVDRIQNE-UHFFFAOYSA-N
Formula:	C15H26
SMILES:	CC1=CCC(C(C)CCCC(C)C)C=C1
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	145.28	kJ/mol	Joback Method
hf	-205.08	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.971		Crippen Method
mcvol	202.750	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	1445.00		NIST Webbook
tb	564.57	K	Joback Method
tc	762.00	K	Joback Method
tf	250.23	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.42	J/molxK	564.57	Joback Method
cpg	534.41	J/molxK	597.47	Joback Method
cpg	554.32	J/molxK	630.38	Joback Method
cpg	573.18	J/molxK	663.28	Joback Method
cpg	591.02	J/molxK	696.19	Joback Method
cpg	607.88	J/molxK	729.09	Joback Method
cpg	623.79	J/molxK	762.00	Joback Method
dvisc	0.0067473	Paxs	250.23	Joback Method
dvisc	0.0021104	Paxs	302.62	Joback Method

dvisc	0.0009302	Paxs	355.01	Joback Method
dvisc	0.0005062	Paxs	407.40	Joback Method
dvisc	0.0003164	Paxs	459.79	Joback Method
dvisc	0.0002177	Paxs	512.18	Joback Method
dvisc	0.0001606	Paxs	564.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R519936&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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