

9,10-Dehydro-ar-curcumene

Inchi:	InChI=1S/C15H20/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h5-11,14H,1-4H3/b7-5-
InchiKey:	UVXCRTURFFRBRL-ALCCZGGFSA-N
Formula:	C15H20
SMILES:	CC(C)=CC=CC(C)c1ccc(C)cc1
Mol. weight [g/mol]:	200.32

Physical Properties

Property code	Value	Unit	Source
gf	327.65	kJ/mol	Joback Method
hf	91.50	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.621		Crippen Method
mcvol	189.850	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	1489.00		NIST Webbook
rinpol	1489.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1900.00		NIST Webbook
tb	582.02	K	Joback Method
tc	799.41	K	Joback Method
tf	258.63	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.85	J/molxK	582.02	Joback Method
cpg	473.18	J/molxK	618.25	Joback Method
cpg	490.36	J/molxK	654.48	Joback Method
cpg	506.46	J/molxK	690.72	Joback Method
cpg	521.56	J/molxK	726.95	Joback Method
cpg	535.72	J/molxK	763.18	Joback Method

Sources

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=R229608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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