

Dihydrorimuene

Inchi:	InChI=1S/C20H34/c1-6-19(4)12-13-20(5)15(14-19)9-10-16-17(20)8-7-11-18(16,2)3/h6,15
InchiKey:	WBIQHNHINYMCJQ-BKXYZSJASA-N
Formula:	C20H34
SMILES:	C=CC1(C)CCC2(C)C(CCC3C2CCCC3(C)C)C1
Mol. weight [g/mol]:	274.48

Physical Properties

Property code	Value	Unit	Source
gf	287.51	kJ/mol	Joback Method
hf	-158.40	kJ/mol	Joback Method
hfus	14.50	kJ/mol	Joback Method
hvap	55.66	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.221		Crippen Method
mcvol	255.780	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1940.00		NIST Webbook
ripol	2154.00		NIST Webbook
ripol	2187.00		NIST Webbook
tb	681.96	K	Joback Method
tc	918.54	K	Joback Method
tf	408.60	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.45	J/molxK	681.96	Joback Method
cpg	816.02	J/molxK	721.39	Joback Method
cpg	843.51	J/molxK	760.82	Joback Method
cpg	870.37	J/molxK	800.25	Joback Method
cpg	897.04	J/molxK	839.68	Joback Method
cpg	923.96	J/molxK	879.11	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=R27299&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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