

Dolabradiene

Inchi: InChI=1S/C20H32/c1-6-18(3)12-13-20(5)16(14-18)10-11-19(4)15(2)8-7-9-17(19)20/h6,16-18,20
InchiKey: GHYZJFFJSPZRIU-WKRFVHVSA-N
Formula: C20H32
SMILES: C=CC1(C)CCC2(C)C(CCC3(C)C(=C)CCCC32)C1
Mol. weight [g/mol]: 272.47
CAS: 3650-13-3

Physical Properties

Property code	Value	Unit	Source
gf	348.30	kJ/mol	Joback Method
hf	-53.82	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	56.13	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.142		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1945.00		NIST Webbook
ripol	2283.00		NIST Webbook
ripol	2283.00		NIST Webbook
ripol	2318.00		NIST Webbook
tb	685.79	K	Joback Method
tc	924.17	K	Joback Method
tf	426.52	K	Joback Method
vc	0.944	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.33	J/mol×K	685.79	Joback Method
cpg	788.39	J/mol×K	725.52	Joback Method
cpg	814.52	J/mol×K	765.25	Joback Method

cpg	840.16	J/mol×K	804.98	Joback Method
cpg	865.78	J/mol×K	844.71	Joback Method
cpg	891.81	J/mol×K	884.44	Joback Method
cpg	918.72	J/mol×K	924.17	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=C3650133&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
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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