

Rosa-5(10),15-diene

Inchi:	InChI=1S/C20H32/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:	XLQFULDKFPTYLT-KHPNHKCMSA-N
Formula:	C20H32
SMILES:	<chem>C=CC1(C)CCC2(C)C3=C(CCC2C1)C(C)(C)CCC3</chem>
Mol. weight [g/mol]:	272.47

Physical Properties

Property code	Value	Unit	Source
gf	313.63	kJ/mol	Joback Method
hf	-82.88	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	57.90	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1917.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2156.00		NIST Webbook
tb	700.42	K	Joback Method
tc	940.52	K	Joback Method
tf	442.88	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.41	J/molxK	700.42	Joback Method
cpg	787.70	J/molxK	740.44	Joback Method
cpg	813.29	J/molxK	780.45	Joback Method
cpg	838.65	J/molxK	820.47	Joback Method
cpg	864.25	J/molxK	860.49	Joback Method
cpg	890.55	J/molxK	900.51	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=R27374&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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