

Dimyrcene II-a

Inchi:	InChI=1S/C20H34/c1-16(2)9-6-11-18(5)20-14-8-13-19(15-20)12-7-10-17(3)4/h9-10,19-20
InchiKey:	AIPIFXVDYDBWHE-UHFFFAOYSA-N
Formula:	C20H34
SMILES:	<chem>C=C(CCC=C(C)C)C1CCCC(CCC=C(C)C)C1</chem>
Mol. weight [g/mol]:	274.48

Physical Properties

Property code	Value	Unit	Source
gf	356.89	kJ/mol	Joback Method
hf	-91.65	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.842		Crippen Method
mcvol	268.900	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
ripol	2219.00		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2219.00		NIST Webbook
tb	676.52	K	Joback Method
tc	877.40	K	Joback Method
tf	264.50	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.38	J/molxK	676.52	Joback Method
cpg	795.96	J/molxK	710.00	Joback Method
cpg	818.21	J/molxK	743.48	Joback Method
cpg	839.20	J/molxK	776.96	Joback Method
cpg	859.01	J/molxK	810.44	Joback Method
cpg	877.71	J/molxK	843.92	Joback Method
cpg	895.38	J/molxK	877.40	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=R407180&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
hvp:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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