Dimyrcene I-a

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

Physical Properties

Property code	Value	Unit	Source
gf	359.95	kJ/mol	Joback Method
hf	-66.62	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.842		Crippen Method
mcvol	268.900	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
ripol	2144.00		NIST Webbook
ripol	2149.00		NIST Webbook
tb	676.88	K	Joback Method
tc	881.24	K	Joback Method
tf	302.36	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.88	J/mol×K	676.88	Joback Method
cpg	792.30	J/mol×K	710.94	Joback Method
cpg	814.58	J/mol×K	745.00	Joback Method
cpg	835.86	J/mol×K	779.06	Joback Method
cpg	856.31	J/mol×K	813.12	Joback Method
cpg	876.05	J/mol×K	847.18	Joback Method
cpg	895.25	J/mol×K	881.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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