Dimyrcene isomer # 2

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

Physical Properties

Property code	Value	Unit	Source
gf	387.99	kJ/mol	Joback Method
hf	0.03	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	59.75	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.762		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	685.69	K	Joback Method
tc	892.56	K	Joback Method
tf	319.88	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.04	J/mol×K	685.69	Joback Method
cpg	765.92	J/mol×K	720.17	Joback Method
cpg	786.77	J/mol×K	754.65	Joback Method
cpg	806.75	J/mol×K	789.12	Joback Method
cpg	826.00	J/mol×K	823.60	Joback Method
cpg	844.69	J/mol×K	858.08	Joback Method
cpg	862.97	J/mol×K	892.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587310&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume