Myrcene dimer

Other names: Dimyrcene
Inchi: InChI=1S/C20H32/c1-16(2)8-6-10-18(5)20-14-12-19(13-15-20)11-7-9-17(3)4/h8-9,12,20H
InchiKey: GJYJYFHBOBUTBY-UHFFFAOYSA-N
Formula: C20H32
SMILES: C=C(CCC=C(C)C)C1CC=C(CCC=C(C)C)CC1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	384.93	kJ/mol	Joback Method
hf	-25.00	kJ/mol	Joback Method
hfus	35.42	kJ/mol	Joback Method
hvap	60.98	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.762		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	1958.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2226.00		NIST Webbook
ripol	2178.00		NIST Webbook
tb	685.33	K	Joback Method
tc	888.68	K	Joback Method
tf	282.02	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.72	J/mol×K	685.33	Joback Method
cpg	769.74	J/mol×K	719.22	Joback Method
cpg	790.51	J/mol×K	753.11	Joback Method
cpg	810.11	J/mol×K	787.00	Joback Method
cpg	828.61	J/mol×K	820.89	Joback Method

cpg	846.10	J/mol×K	854.78	Joback Method
cpg	862.66	J/mol×K	888.68	Joback Method

Sources

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=R291242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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