Sesquicalamene

Inchi: InChI=1S/C20H30/c1-14(2)7-6-8-17-10-12-18(15(3)4)20-13-16(5)9-11-19(17)20/h7,10,12
InchiKey: FXLZQAKRGHXOSS-UHFFFAOYSA-N
Formula: C20H30
SMILES: CC(C)=CCCc1ccc(C(C)C)c2c1CCC(C)C2
Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	318.92	kJ/mol	Joback Method
hf	-85.22	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.834		Crippen Method
mcvol	253.740	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
ripol	1675.00		NIST Webbook
tb	713.23	K	Joback Method
tc	926.82	K	Joback Method
tf	359.52	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.83	J/mol×K	713.23	Joback Method
cpg	756.03	J/mol×K	748.83	Joback Method
cpg	775.98	J/mol×K	784.43	Joback Method
cpg	794.76	J/mol×K	820.03	Joback Method
cpg	812.46	J/mol×K	855.62	Joback Method
cpg	829.14	J/mol×K	891.22	Joback Method
cpg	844.90	J/mol×K	926.82	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=R635013&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume