Dimer of «alpha»-phellandrene 1

Inchi: InChI=1S/C20H32/c1-13(2)16-8-7-15(5)17-18(16)20(14(3)4)11-9-19(17,6)10-12-20/h7,9,
InchiKey: YLRZSKBKTCAWKB-UHFFFAOYSA-N
Formula: C20H32
SMILES: CC1=CCC(C(C)C)C2C1C1(C)C=CC2(C(C)C)CC1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	282.48	kJ/mol	Joback Method
hf	-172.88	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	57.92	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.853		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinpol	1795.00		NIST Webbook
tb	683.59	K	Joback Method
tc	906.97	K	Joback Method
tf	381.78	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.99	J/mol×K	683.59	Joback Method
cpg	785.89	J/mol×K	720.82	Joback Method
cpg	809.73	J/mol×K	758.05	Joback Method
cpg	832.79	J/mol×K	795.28	Joback Method
cpg	855.38	J/mol×K	832.51	Joback Method
cpg	877.80	J/mol×K	869.74	Joback Method
cpg	900.33	J/mol×K	906.97	Joback Method

Sources

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=R286389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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