«alpha»-Phellandrene, dimer

Inchi: InChI=1S/C20H32/c1-13(2)15-7-9-19(5)17(11-15)18-12-16(14(3)4)8-10-20(18,19)6/h7-10
InchiKey: YNQNZPAXEWELDZ-UHFFFAOYSA-N
Formula: C20H32
SMILES: CC(C)C1C=CC2(C)C(C1)C1CC(C(C)C)C=CC12C
Mol. weight [g/mol]: 272.47
CAS: 7350-11-0

Physical Properties

Property code	Value	Unit	Source
gf	284.40	kJ/mol	Joback Method
hf	-181.75	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	56.95	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.709		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1801.40		NIST Webbook
tb	673.94	K	Joback Method
tc	896.52	K	Joback Method
tf	365.02	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.91	J/mol×K	673.94	Joback Method
cpg	787.50	J/mol×K	711.04	Joback Method
cpg	811.89	J/mol×K	748.13	Joback Method
cpg	835.40	J/mol×K	785.23	Joback Method
cpg	858.30	J/mol×K	822.33	Joback Method
cpg	880.89	J/mol×K	859.42	Joback Method
cpg	903.47	J/mol×K	896.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7350110&Units=SI

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