«alpha»-Sesquiphellandrene

Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8-10,14-15H,5,7,11H2,1-
InchiKey: KKOXKGNSUHTUBV-CABCVRRESA-N
Formula: C15H24
SMILES: CC(C)=CCCC(C)C1C=CC(C)=CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	219.39	kJ/mol	Joback Method
hf	-92.37	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	50.31	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1526.00		NIST Webbook
tb	569.05	K	Joback Method
tc	774.33	K	Joback Method
tf	246.19	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.43	J/mol×K	569.05	Joback Method
cpg	514.99	J/mol×K	603.26	Joback Method
cpg	534.40	J/mol×K	637.48	Joback Method
cpg	552.71	J/mol×K	671.69	Joback Method
cpg	569.96	J/mol×K	705.90	Joback Method
cpg	586.22	J/mol×K	740.11	Joback Method
cpg	601.53	J/mol×K	774.33	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=R519996&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