«delta»-patchoulene

Inchi: InChI=1S/C16H28/c1-12(2)6-7-14-9-8-13-10-11-16(14,5)15(13,3)4/h9,12-13H,6-8,10-11H
InchiKey: BLLLUIMYYWMBGY-UHFFFAOYSA-N
Formula: C16H28
SMILES: CC(C)CCC1=CCC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 220.39

Physical Properties

Property code	Value	Unit	Source
gf	180.34	kJ/mol	Joback Method
hf	-189.12	kJ/mol	Joback Method
hfus	15.05	kJ/mol	Joback Method
hvap	49.34	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.195		Crippen Method
mcvol	210.280	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1452.00		NIST Webbook
ripol	1627.00		NIST Webbook
tb	587.01	K	Joback Method
tc	797.84	K	Joback Method
tf	340.76	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.02	J/mol×K	587.01	Joback Method
cpg	591.16	J/mol×K	622.15	Joback Method
cpg	612.03	J/mol×K	657.29	Joback Method
cpg	631.86	J/mol×K	692.42	Joback Method
cpg	650.87	J/mol×K	727.56	Joback Method
cpg	669.29	J/mol×K	762.70	Joback Method
cpg	687.34	J/mol×K	797.84	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=R238201&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume