2,2,4a,6a,6b,9-Hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,12b,13,14b-tetradecahydro-picene

Inchi: InChI=1S/C28H40/c1-19-8-7-9-21-20(19)12-13-27(5)22(21)10-11-23-24-18-25(2,3)14-15

InchiKey: LLJZJNHOOHQEGE-UHFFFAOYSA-N

Formula: C28H40

SMILES: Cc1cccc2c1CCC1(C)C2CC=C2C3CC(C)(C)CCC3(C)CCC21C

Mol. weight [g/mol]: 376.62

Physical Properties

Property code	Value	Unit	Source
gf	455.58	kJ/mol	Joback Method
hf	-74.51	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	7.994		Crippen Method
mcvol	333.880	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	3013.08		NIST Webbook
tb	916.48	K	Joback Method
tc	1172.05	K	Joback Method
tf	614.86	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.22	J/mol×K	916.48	Joback Method
cpg	1232.78	J/mol×K	959.07	Joback Method
cpg	1275.36	J/mol×K	1001.67	Joback Method
cpg	1321.75	J/mol×K	1044.26	Joback Method
cpg	1372.72	J/mol×K	1086.86	Joback Method
cpg	1429.05	J/mol×K	1129.45	Joback Method
cpg	1491.54	J/mol×K	1172.05	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=U146457&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume