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

Inchi: InChI=1S/C28H40/c1-18-12-14-26(4)16-17-28(6)24(25(26)20(18)3)11-10-23-22-9-7-8-19

InchiKey: CPRUTHPUWILGGA-UHFFFAOYSA-N

Formula: C28H40

SMILES: Cc1cccc2c1CCC1(C)C2CC=C2C3C(C)C(C)CCC3(C)CCC21C

Mol. weight [g/mol]: 376.62

Physical Properties

Property code	Value	Unit	Source
gf	453.36	kJ/mol	Joback Method
hf	-110.09	kJ/mol	Joback Method
hfus	30.83	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	7.850		Crippen Method
mcvol	333.880	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
rinpol	2970.25		NIST Webbook
tb	911.57	K	Joback Method
tc	1160.27	K	Joback Method
tf	586.72	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1196.01	J/mol×K	911.57	Joback Method
cpg	1231.18	J/mol×K	953.02	Joback Method
cpg	1267.91	J/mol×K	994.47	Joback Method
cpg	1306.79	J/mol×K	1035.92	Joback Method
cpg	1348.41	J/mol×K	1077.37	Joback Method
cpg	1393.34	J/mol×K	1118.82	Joback Method
cpg	1442.17	J/mol×K	1160.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R179667&Units=SI
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

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