

7-Isopropyl-1,1,4a-trimethyl-tetradecahydro-phen

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H36/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h14-1

STIVVCHBLMGYSL-UHFFFAOYSA-N

C20H36

CC(C)C1CCC2C(CCC3C(C)(C)CCCC23C)C1

276.50

Physical Properties

Property code	Value	Unit	Source
gf	202.72	kJ/mol	Joback Method
hf	-304.35	kJ/mol	Joback Method
hfus	18.55	kJ/mol	Joback Method
hvap	57.10	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	6.301		Crippen Method
mcvol	260.080	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	684.60	K	Joback Method
tc	912.76	K	Joback Method
tf	371.46	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.11	J/mol×K	684.60	Joback Method
cpg	845.19	J/mol×K	722.63	Joback Method
cpg	872.91	J/mol×K	760.65	Joback Method
cpg	899.54	J/mol×K	798.68	Joback Method
cpg	925.39	J/mol×K	836.70	Joback Method
cpg	950.75	J/mol×K	874.73	Joback Method
cpg	975.90	J/mol×K	912.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490370&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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