4-Isopropyl-1-methyl-3-[1,5,9-trimethyl-1-(4-methy

Inchi: InChI=1S/C30H56/c1-10-25(6)16-12-20-30(9,21-13-17-26(7)15-11-14-23(2)3)29-22-27(8

InchiKey: VRKPWMBSRMUFHZ-UHFFFAOYSA-N

Formula: C30H56

SMILES: C=C(C)C1CCC(C)=CC1C(C)(CCCC(C)CC)CCCC(C)CCCC(C)C

Mol. weight [g/mol]: 416.77

Physical Properties

Property code	Value	Unit	Source
gf	313.60	kJ/mol	Joback Method
hf	-491.19	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-10.53		Crippen Method
logp	10.390		Crippen Method
mcvol	414.100	ml/mol	McGowan Method
pc	687.09	kPa	Joback Method
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook
tb	896.83	K	Joback Method
tc	1099.61	K	Joback Method
tf	385.98	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.80	J/mol×K	896.83	Joback Method
cpg	1452.54	J/mol×K	930.63	Joback Method
cpg	1475.79	J/mol×K	964.42	Joback Method
cpg	1497.64	J/mol×K	998.22	Joback Method
cpg	1518.17	J/mol×K	1032.02	Joback Method
cpg	1537.48	J/mol×K	1065.81	Joback Method
cpg	1555.67	J/mol×K	1099.61	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=R507656&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