

4-Isopropenyl-1-methyl-3-[1,5,9-trimethyl-1-(4-met

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C30H50/c1-10-25(6)16-12-20-30(9,21-13-17-26(7)15-11-14-23(2)3)29-22-27(8

ZJVXDMICLAHVAH-YZSQISJMSA-N

C30H50

C=CC(C)CCCC(C)(CCC=C(C)CCC=C(C)C)C1C=C(C)CCC1C(=C)C

410.72

Physical Properties

Property code	Value	Unit	Source
gf	549.66	kJ/mol	Joback Method
hf	-140.34	kJ/mol	Joback Method
hfus	50.17	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-10.58		Crippen Method
logp	10.007		Crippen Method
mcvol	401.200	ml/mol	McGowan Method
pc	740.43	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	902.47	K	Joback Method
tc	1110.64	K	Joback Method
tf	376.14	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.02	J/mol×K	902.47	Joback Method
cpg	1367.66	J/mol×K	937.16	Joback Method
cpg	1390.08	J/mol×K	971.86	Joback Method
cpg	1411.41	J/mol×K	1006.55	Joback Method
cpg	1431.77	J/mol×K	1041.25	Joback Method
cpg	1451.29	J/mol×K	1075.94	Joback Method
cpg	1470.11	J/mol×K	1110.64	Joback Method

Sources

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=R507641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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