

2,6,10,14,18-Pentamethyl-13-(3-methyl-pent-4-enyl)-1-ene

Inchi: InChI=1S/C30H52/c1-10-26(6)20-22-30(29(9)19-12-15-25(4)5)23-21-28(8)18-13-17-27(7)
InchiKey: BNYPZWFLESHHNE-WVSZGKPXSA-N
Formula: C30H52
SMILES: C=CC(C)CC=C(CC=C(C)CCC=C(C)CCC=C(C)C)C(C)CCCC(C)C
Mol. weight [g/mol]: 412.73

Physical Properties

Property code	Value	Unit	Source
gf	568.92	kJ/mol	Joback Method
hf	-123.22	kJ/mol	Joback Method
hfus	57.17	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Joback Method
log10ws	-10.92		Crippen Method
logp	10.397		Crippen Method
mcvol	412.060	ml/mol	McGowan Method
pc	691.07	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
rinpol	2505.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	897.32	K	Joback Method
tc	1099.61	K	Joback Method
tf	304.94	K	Joback Method
vc	1.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.52	J/molxK	897.32	Joback Method
cpg	1371.19	J/molxK	931.04	Joback Method
cpg	1393.90	J/molxK	964.75	Joback Method
cpg	1415.77	J/molxK	998.47	Joback Method
cpg	1436.93	J/molxK	1032.18	Joback Method

cpg	1457.51	J/mol×K	1065.90	Joback Method
cpg	1477.64	J/mol×K	1099.61	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=R507507&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
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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