

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

Inchi:
trans

InChI=1S/C30H50/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:

JCWJDRJIYCBBNM-OGXFWODGSA-N

Formula:

C30H50

SMILES:

C=CC(C)CC=C(CC=C(C)CCC=C(C)CCC=C(C)C)C(C)CCC=C(C)C

Mol. weight [g/mol]:

410.72

Physical Properties

Property code	Value	Unit	Source
gf	643.03	kJ/mol	Joback Method
hf	-10.51	kJ/mol	Joback Method
hfus	59.59	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-11.02		Crippen Method
logp	10.317		Crippen Method
mcvol	407.760	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
rinpol	2617.00		NIST Webbook
tb	901.80	K	Joback Method
tc	1106.06	K	Joback Method
tf	300.90	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.19	J/molxK	901.80	Joback Method
cpg	1343.53	J/molxK	935.84	Joback Method
cpg	1366.03	J/molxK	969.89	Joback Method
cpg	1387.85	J/molxK	1003.93	Joback Method
cpg	1409.11	J/molxK	1037.98	Joback Method
cpg	1429.97	J/molxK	1072.02	Joback Method
cpg	1450.57	J/molxK	1106.06	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=R501514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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