

2,6(E)-Heptadecadiene, 2,6,12,16-tetramethyl-11-(3-methyl-4-pentenyliden)

Inchi: InChI=1S/C27H48/c1-9-24(6)20-21-27(26(8)18-13-15-23(4)5)19-11-10-16-25(7)17-12-14

InchiKey: QWEORNKNGOBVIS-XRBBYRFDSA-N

Formula: C27H48

SMILES: C=CC(C)CC=C(CCCC=C(C)CCC=C(C)C)C(C)CCCC(C)C

Mol. weight [g/mol]: 372.67

Physical Properties

Property code	Value	Unit	Source
gf	471.99	kJ/mol	Joback Method
hf	-168.73	kJ/mol	Joback Method
hfus	50.51	kJ/mol	Joback Method
hvap	73.98	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.450		Crippen Method
mcvol	374.090	ml/mol	McGowan Method
pc	783.31	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
tb	824.64	K	Joback Method
tc	1015.09	K	Joback Method
tf	290.17	K	Joback Method
vc	1.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.66	J/mol×K	824.64	Joback Method
cpg	1202.27	J/mol×K	856.38	Joback Method
cpg	1223.83	J/mol×K	888.12	Joback Method
cpg	1244.44	J/mol×K	919.86	Joback Method
cpg	1264.18	J/mol×K	951.60	Joback Method
cpg	1283.15	J/mol×K	983.35	Joback Method
cpg	1301.44	J/mol×K	1015.09	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=R507745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvpap:	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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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