2,6(E),15-Heptadecatriene, 2,6,16-trimethyl-12-methylene-11-(3-methyl-4-pent

Inchi: InChI=1S/C27H46/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: ZWDJPIIGWKVHAH-PCLIKHOPSA-N

Formula: C27H46

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

Mol. weight [g/mol]: 370.65

Physical Properties

Property code	Value	Unit	Source
gf	553.72	kJ/mol	Joback Method
hf	-47.81	kJ/mol	Joback Method
hfus	51.45	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	9.370		Crippen Method
mcvol	369.790	ml/mol	McGowan Method
pc	800.69	kPa	Joback Method
rinpol	2174.00		NIST Webbook
tb	821.64	K	Joback Method
tc	1012.71	K	Joback Method
tf	289.45	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.16	J/mol×K	821.64	Joback Method
cpg	1173.27	J/mol×K	853.48	Joback Method
cpg	1194.37	J/mol×K	885.33	Joback Method
cpg	1214.56	J/mol×K	917.17	Joback Method
cpg	1233.94	J/mol×K	949.02	Joback Method
cpg	1252.60	J/mol×K	980.86	Joback Method
cpg	1270.64	J/mol×K	1012.71	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=R507730&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume