1-[(E)-1,4,7,10,11,14,15-heptamethyl-4-vinyl-5-hexa
Isomer # 1

InchI: InChI=1S/C34H64/c1-13-34(12,23-21-30(8)32-19-18-31(9)33(10,11)24-32)22-20-26(4)14
InchiKey: MXZICHDKCVIUPH-LSDHQDQOSA-N
Formula: C34H64
SMILES: C=CC(C)(C=CC(C)CCC(C)C(C)CCC(C)C(C)C)CCC(C)C1CCC(C)C(C)(C)C1
Mol. weight [g/mol]: 472.87

Physical Properties

Property code	Value	Unit	Source
gf	395.20	kJ/mol	Joback Method
hf	-513.99	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-11.24		Crippen Method
logp	11.374		Crippen Method
mcvol	470.460	ml/mol	McGowan Method
pc	584.29	kPa	Joback Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook
tb	982.74	K	Joback Method
tc	1203.15	K	Joback Method
tf	401.32	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1710.18	J/mol×K	982.74	Joback Method
cpg	1740.97	J/mol×K	1019.47	Joback Method
cpg	1771.10	J/mol×K	1056.21	Joback Method
cpg	1800.79	J/mol×K	1092.94	Joback Method
cpg	1830.28	J/mol×K	1129.68	Joback Method
cpg	1859.80	J/mol×K	1166.41	Joback Method
cpg	1889.59	J/mol×K	1203.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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