(6E,11E,16E)-2,3,6,10,13,17,20,21-octamethyl-10-v
Isomer # 4

Inchi: InChI=1S/C32H54/c1-12-32(11,23-14-17-28(7)19-21-31(10)26(4)5)24-22-29(8)16-13-15-

InchiKey: YIERDWVPDSIPLW-PTFXNVDKSA-N

Formula: C32H54

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

Mol. weight [g/mol]: 438.77

Physical Properties

Property code	Value	Unit	Source
gf	684.06	kJ/mol	Joback Method
hf	-39.61	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	82.55	kJ/mol	Joback Method
log10ws	-11.37		Crippen Method
logp	10.809		Crippen Method
mcvol	435.940	ml/mol	McGowan Method
pc	642.55	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	929.05	K	Joback Method
tc	1137.84	K	Joback Method
tf	331.46	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.63	J/mol×K	929.05	Joback Method
cpg	1470.80	J/mol×K	963.85	Joback Method
cpg	1494.07	J/mol×K	998.65	Joback Method
cpg	1516.60	J/mol×K	1033.44	Joback Method
cpg	1538.55	J/mol×K	1068.24	Joback Method
cpg	1560.09	J/mol×K	1103.04	Joback Method
cpg	1581.37	J/mol×K	1137.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586540&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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