(7E)-2-(3,4-dimethylpentyl)-3,6,9,12,16,17-hexamet

Inchi: InChI=1S/C34H60/c1-14-34(13,24-22-33(12)32(11)20-18-29(8)26(4)5)23-21-27(6)15-16-

InchiKey: GNKJQNWBNLBMNN-XTQSDGFTSA-N

Formula: C34H60

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

Mol. weight [g/mol]: 468.84

Physical Properties

Property code	Value	Unit	Source
gf	629.53	kJ/mol	Joback Method
hf	-195.95	kJ/mol	Joback Method
hfus	46.42	kJ/mol	Joback Method
hvap	85.17	kJ/mol	Joback Method
log10ws	-11.63		Crippen Method
logp	11.381		Crippen Method
mcvol	468.420	ml/mol	McGowan Method
pc	572.33	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	961.97	K	Joback Method
tc	1178.28	K	Joback Method
tf	331.36	K	Joback Method
vc	1.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.73	J/mol×K	961.97	Joback Method
cpg	1631.31	J/mol×K	998.02	Joback Method
cpg	1655.72	J/mol×K	1034.07	Joback Method
cpg	1679.13	J/mol×K	1070.13	Joback Method
cpg	1701.71	J/mol×K	1106.18	Joback Method
cpg	1723.61	J/mol×K	1142.23	Joback Method
cpg	1745.00	J/mol×K	1178.28	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586575&Units=SI

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