

(11E)-2,3,7,10,13,20,21-heptamethyl-6,17-dimethyl

Inchi:

InChI=1S/C34H58/c1-13-29(7)31(9)19-17-27(5)16-15-24-34(12,14-2)25-23-28(6)18-20-3

InchiKey:

UOKGMRGCUVYZIE-NEVRGKPLSA-N

Formula:

C34H58

SMILES:

C=CC(C)(C=CC(C)CCC(C)C(=C)CCC(C)C(=C)C)CCCC(=C)CCC(C)C(C)=CC

Mol. weight [g/mol]:

466.82

Physical Properties

Property code	Value	Unit	Source
gf	706.08	kJ/mol	Joback Method
hf	-77.96	kJ/mol	Joback Method
hfus	52.35	kJ/mol	Joback Method
hvap	85.99	kJ/mol	Joback Method
log10ws	-11.97		Crippen Method
logp	11.445		Crippen Method
mcvol	464.120	ml/mol	McGowan Method
pc	583.73	kPa	Joback Method
rinpol	2713.00		NIST Webbook
tb	966.89	K	Joback Method
tc	1184.13	K	Joback Method
tf	342.32	K	Joback Method
vc	1.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.47	J/molxK	966.89	Joback Method
cpg	1602.88	J/molxK	1003.10	Joback Method
cpg	1627.33	J/molxK	1039.30	Joback Method
cpg	1651.00	J/molxK	1075.51	Joback Method
cpg	1674.06	J/molxK	1111.72	Joback Method
cpg	1696.69	J/molxK	1147.92	Joback Method
cpg	1719.09	J/molxK	1184.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R586397&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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