

isotactic-2,4,6,8,10,12-Hexaethyl-1,12-tridecadiene

Inchi:	InChI=1S/C19H36/c1-14(2)9-16(5)11-18(7)13-19(8)12-17(6)10-15(3)4/h16-19H,1,3,9-13H
InchiKey:	AEWAVWPWBCLUIU-UHFFFAOYSA-N
Formula:	C19H36
SMILES:	C=C(C)CC(C)CC(C)CC(C)CC(C)CC(=C)C
Mol. weight [g/mol]:	264.49

Physical Properties

Property code	Value	Unit	Source
gf	257.92	kJ/mol	Joback Method
hf	-225.33	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	6.633		Crippen Method
mvol	269.970	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	625.48	K	Joback Method
tc	801.88	K	Joback Method
tf	212.45	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.29	J/mol×K	625.48	Joback Method
cpg	757.68	J/mol×K	654.88	Joback Method
cpg	778.07	J/mol×K	684.28	Joback Method
cpg	797.50	J/mol×K	713.68	Joback Method
cpg	815.99	J/mol×K	743.08	Joback Method
cpg	833.61	J/mol×K	772.48	Joback Method
cpg	850.37	J/mol×K	801.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R628510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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