

heterotactic-2,4,6,8-Tetramethyl-1-undecene

Inchi:	InChI=1S/C15H28/c1-7-8-13(4)10-15(6)11-14(5)9-12(2)3/h7,13-15H,1-2,8-11H2,3-6H3
InchiKey:	DGCZFTURLLFENG-UHFFFAOYSA-N
Formula:	C15H28
SMILES:	<chem>C=CCC(C)CC(C)CC(C)CC(=C)C</chem>
Mol. weight [g/mol]:	208.38

Physical Properties

Property code	Value	Unit	Source
gf	235.23	kJ/mol	Joback Method
hf	-127.70	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	5.217		Crippen Method
mvol	213.610	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1320.00		NIST Webbook
tb	534.52	K	Joback Method
tc	710.57	K	Joback Method
tf	196.33	K	Joback Method
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.41	J/mol×K	534.52	Joback Method
cpg	537.66	J/mol×K	563.86	Joback Method
cpg	556.04	J/mol×K	593.20	Joback Method
cpg	573.58	J/mol×K	622.55	Joback Method
cpg	590.30	J/mol×K	651.89	Joback Method
cpg	606.24	J/mol×K	681.23	Joback Method
cpg	621.43	J/mol×K	710.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R628481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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