

2,4,4,6,6,8,8-Heptamethyl-2-nonene

Inchi:	InChI=1S/C16H32/c1-13(2)10-15(6,7)12-16(8,9)11-14(3,4)5/h10H,11-12H2,1-9H3
InchiKey:	YJSQJYADFSVLHZ-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	CC(C)=CC(C)(C)CC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	224.43
CAS:	39761-73-4

Physical Properties

Property code	Value	Unit	Source
gf	164.03	kJ/mol	Joback Method
hf	-292.39	kJ/mol	Joback Method
hfus	13.85	kJ/mol	Joback Method
hvap	47.36	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.831		Crippen Method
mcvol	232.000	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	232.30		NIST Webbook
rinpol	232.30		NIST Webbook
tb	559.83	K	Joback Method
tc	754.26	K	Joback Method
tf	258.30	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.71	J/mol×K	559.83	Joback Method
cpg	623.24	J/mol×K	592.24	Joback Method
cpg	644.38	J/mol×K	624.64	Joback Method
cpg	664.23	J/mol×K	657.05	Joback Method
cpg	682.88	J/mol×K	689.45	Joback Method
cpg	700.41	J/mol×K	721.86	Joback Method
cpg	716.93	J/mol×K	754.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39761734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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