

Hexadecane, 3,7,11-trimethyl

Other names:	3,7,11-trimethylhexadecane
Inchi:	InChI=1S/C19H40/c1-6-8-9-12-18(4)15-11-16-19(5)14-10-13-17(3)7-2/h17-19H,6-16H2,1
InchiKey:	FCGOBFXOCBSQIP-UHFFFAOYSA-N
Formula:	C19H40
SMILES:	CCCCC(C)CCCC(C)CCCC(C)CC
Mol. weight [g/mol]:	268.52

Physical Properties

Property code	Value	Unit	Source
gf	101.78	kJ/mol	Joback Method
hf	-451.33	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	56.72	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	7.226		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	1755.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1754.00		NIST Webbook
tb	632.80	K	Joback Method
tc	798.17	K	Joback Method
tf	258.89	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.31	J/mol×K	632.80	Joback Method
cpg	803.70	J/mol×K	660.36	Joback Method
cpg	824.19	J/mol×K	687.92	Joback Method

cpg	843.79	J/molxK	715.49	Joback Method
cpg	862.54	J/molxK	743.05	Joback Method
cpg	880.46	J/molxK	770.61	Joback Method
cpg	897.59	J/molxK	798.17	Joback Method
dvisc	0.0137841	Paxs	258.89	Joback Method
dvisc	0.0026251	Paxs	321.21	Joback Method
dvisc	0.0008570	Paxs	383.53	Joback Method
dvisc	0.0003826	Paxs	445.84	Joback Method
dvisc	0.0002081	Paxs	508.16	Joback Method
dvisc	0.0001294	Paxs	570.48	Joback Method
dvisc	0.0000883	Paxs	632.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R12163&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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