

1-Tridecene, 3,7,11-trimethyl

Inchi:	InChI=1S/C16H32/c1-6-14(3)10-8-12-16(5)13-9-11-15(4)7-2/h6,14-16H,1,7-13H2,2-5H3
InchiKey:	SMXPEKNRQAAHID-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	C=CC(C)CCCC(C)CCCC(C)CC
Mol. weight [g/mol]:	224.43

Physical Properties

Property code	Value	Unit	Source
gf	164.36	kJ/mol	Joback Method
hf	-263.98	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.831		Crippen Method
mcvol	232.000	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinsol	1460.00		NIST Webbook
tb	560.84	K	Joback Method
tc	730.04	K	Joback Method
tf	223.32	K	Joback Method
vc	0.894	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.57	J/molxK	560.84	Joback Method
cpg	611.43	J/molxK	589.04	Joback Method
cpg	630.44	J/molxK	617.24	Joback Method
cpg	648.63	J/molxK	645.44	Joback Method
cpg	666.02	J/molxK	673.64	Joback Method
cpg	682.64	J/molxK	701.84	Joback Method
cpg	698.51	J/molxK	730.04	Joback Method
dvisc	0.0197453	Paxs	223.32	Joback Method
dvisc	0.0036777	Paxs	279.57	Joback Method

dvisc	0.0012028	Paxs	335.83	Joback Method
dvisc	0.0005421	Paxs	392.08	Joback Method
dvisc	0.0002985	Paxs	448.33	Joback Method
dvisc	0.0001877	Paxs	504.59	Joback Method
dvisc	0.0001295	Paxs	560.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47102&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

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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