Tridecane, 3-methyl-

Other names:	3-Methyltridecane
	Tridecane, 3-methyl-
Inchi:	InChI=1S/C14H30/c1-4-6-7-8-9-10-11-12-13-14(3)5-2/h14H,4-13H2,1-3H3
InchiKey:	NLHRRMKILFRDGV-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCCCCCCCCCC(C)CC
Mol. weight [g/mol]:	198.39
CAS:	6418-41-3

Physical Properties

Property code	Value	Unit	Source
gf	64.56	kJ/mol	Joback Method
hf	-337.57	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	46.37	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.563		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	1371.90		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.23		NIST Webbook
rinpol	1371.66		NIST Webbook
rinpol	1371.68		NIST Webbook
rinpol	1370.88		NIST Webbook
rinpol	1371.14		NIST Webbook
rinpol	1371.32		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1372.30		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1375.00		NIST Webbook

rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.66		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1369.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1366.00		NIST Webbook
tb	519.28	K	Joback Method
tc	681.76	K	Joback Method
tf	235.70 ± 2.00	K	NIST Webbook
tf	235.70 ± 2.00	K	NIST Webbook
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.07	J/mol×K	519.28	Joback Method
cpg	524.54	J/mol×K	546.36	Joback Method
cpg	542.30	J/mol×K	573.44	Joback Method
cpg	559.36	J/mol×K	600.52	Joback Method
cpg	575.74	J/mol×K	627.60	Joback Method
cpg	591.46	J/mol×K	654.68	Joback Method
cpg	606.55	J/mol×K	681.76	Joback Method
dvisc	0.0090478	Pa×s	232.54	Joback Method
dvisc	0.0026666	Pa×s	280.33	Joback Method
dvisc	0.0011218	Pa×s	328.12	Joback Method
dvisc	0.0005882	Pa×s	375.91	Joback Method
dvisc	0.0003567	Pa×s	423.70	Joback Method
dvisc	0.0002394	Pa×s	471.49	Joback Method
dvisc	0.0001730	Pa×s	519.28	Joback Method
hvapt	55.10	kJ/mol	455.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42633e+01
Coeff. B	-4.01636e+03
Coeff. C	-1.05430e+02
Temperature range (K), min.	392.81
Temperature range (K), max.	554.09

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6418413&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume