

Tetradecane, 3-methyl-

Other names:	3-Methyltetradecane
Inchi:	InChI=1S/C15H32/c1-4-6-7-8-9-10-11-12-13-14-15(3)5-2/h15H,4-14H2,1-3H3
InchiKey:	HXUYUZCPGPKNGS-UHFFFAOYSA-N
Formula:	C15H32
SMILES:	CCCCCCCCCCCC(C)CC
Mol. weight [g/mol]:	212.41
CAS:	18435-22-8

Physical Properties

Property code	Value	Unit	Source
gf	72.98	kJ/mol	Joback Method
hf	-358.21	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.953		Crippen Method
mcvol	222.210	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	1471.07		NIST Webbook
rinpol	1471.08		NIST Webbook
rinpol	1471.21		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1472.50		NIST Webbook
rinpol	1471.39		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1471.79		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	542.16	K	Joback Method

tc	703.93	K	Joback Method
tf	237.20 ± 2.00	K	NIST Webbook
vc	0.870	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.59	J/mol×K	703.93	Joback Method
cpg	646.08	J/mol×K	676.97	Joback Method
cpg	629.92	J/mol×K	650.00	Joback Method
cpg	613.07	J/mol×K	623.04	Joback Method
cpg	595.52	J/mol×K	596.08	Joback Method
cpg	577.24	J/mol×K	569.12	Joback Method
cpg	558.22	J/mol×K	542.16	Joback Method
dvisc	0.0083877	Paxs	243.81	Joback Method
dvisc	0.0001577	Paxs	542.16	Joback Method
dvisc	0.0002189	Paxs	492.43	Joback Method
dvisc	0.0003270	Paxs	442.71	Joback Method
dvisc	0.0005409	Paxs	392.99	Joback Method
dvisc	0.0010352	Paxs	343.26	Joback Method
dvisc	0.0024681	Paxs	293.53	Joback Method
hvapt	58.40	kJ/mol	470.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42836e+01
Coeff. B	-4.13364e+03
Coeff. C	-1.11770e+02
Temperature range (K), min.	407.11
Temperature range (K), max.	572.49

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18435228&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/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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