Pentadecane, 4-methyl-

Other names: 4-Methylpentadecane
Inchi: InChI=1S/C16H34/c1-4-6-7-8-9-10-11-12-13-15-16(3)14-5-2/h16H,4-15H2,1-3H3
InchiKey: ODDVOCXSLXTIIU-UHFFFAOYSA-N
Formula: C16H34
SMILES: CCCCCCCCCCCC(C)CCC
Mol. weight [g/mol]: 226.44
CAS: 2801-87-8

Physical Properties

Property code	Value	Unit	Source
gf	81.40	kJ/mol	Joback Method
hf	-378.85	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.344		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	1557.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1556.00		NIST Webbook
ripol	1555.00		NIST Webbook
tb	565.04	K	Joback Method
tc	726.28	K	Joback Method
tf	250.00 ± 2.00	K	NIST Webbook
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/mol×K	565.04	Joback Method
cpg	631.47	J/mol×K	591.91	Joback Method

cpg	650.21	J/mol×K	618.79	Joback Method
cpg	668.20	J/mol×K	645.66	Joback Method
cpg	685.47	J/mol×K	672.53	Joback Method
cpg	702.03	J/mol×K	699.40	Joback Method
cpg	717.90	J/mol×K	726.28	Joback Method
dvisc	0.0077044	Pa×s	255.08	Joback Method
dvisc	0.0022640	Pa×s	306.74	Joback Method
dvisc	0.0009470	Pa×s	358.40	Joback Method
dvisc	0.0004934	Pa×s	410.06	Joback Method
dvisc	0.0002974	Pa×s	461.72	Joback Method
dvisc	0.0001985	Pa×s	513.38	Joback Method
dvisc	0.0001427	Pa×s	565.04	Joback Method
hvapt	57.80	kJ/mol	482.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73871e+01
Coeff. B	-7.11088e+03
Coeff. C	4.00100e+00
Temperature range (K), min.	411.85
Temperature range (K), max.	584.86

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2801878&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