

3-Hexadecyne

Inchi:	InChI=1S/C16H30/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-5,7,9-16H2,1-2H3
InchiKey:	HRFPRVYNMNOAQO-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	CCC#CCCCCCCCCCCCC
Mol. weight [g/mol]:	222.41
CAS:	61886-62-2

Physical Properties

Property code	Value	Unit	Source
gf	286.64	kJ/mol	Joback Method
hf	-101.27	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.711		Crippen Method
mcvol	227.700	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
tb	574.48	K	Joback Method
tc	749.14	K	Joback Method
tf	376.18	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.26	J/mol×K	574.48	Joback Method
cpg	595.18	J/mol×K	603.59	Joback Method
cpg	613.30	J/mol×K	632.70	Joback Method
cpg	630.66	J/mol×K	661.81	Joback Method
cpg	647.27	J/mol×K	690.92	Joback Method
cpg	663.15	J/mol×K	720.03	Joback Method
cpg	678.34	J/mol×K	749.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56840e+01
Coeff. B	-5.09200e+03
Coeff. C	-9.65940e+01
Temperature range (K), min.	427.32
Temperature range (K), max.	587.51

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61886622&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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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