3-Hexadecene

Inchi: InChI=1S/C16H32/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h5,7H,3-4,6,8-16H2,1-2H3
InchiKey: QIZDLUWRENVVJW-UHFFFAOYSA-N
Formula: C16H32
SMILES: CCC=CCCCCCCCCCCCC
Mol. weight [g/mol]: 224.43
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	164.06	kJ/mol	Joback Method
hf	-256.35	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.264		Crippen Method
mcvol	232.000	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	1604.00		NIST Webbook
tb	569.64	K	Joback Method
tc	733.96	K	Joback Method
tf	265.00	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.58	J/mol×K	569.64	Joback Method
cpg	612.46	J/mol×K	597.03	Joback Method
cpg	630.57	J/mol×K	624.41	Joback Method
cpg	647.91	J/mol×K	651.80	Joback Method
cpg	664.52	J/mol×K	679.18	Joback Method
cpg	680.43	J/mol×K	706.57	Joback Method
cpg	695.67	J/mol×K	733.96	Joback Method
dvisc	0.0048369	Pa×s	265.00	Joback Method

dvisc	0.0016294	Pa×s	315.77	Joback Method
dvisc	0.0007420	Pa×s	366.55	Joback Method
dvisc	0.0004092	Pa×s	417.32	Joback Method
dvisc	0.0002567	Pa×s	468.09	Joback Method
dvisc	0.0001765	Pa×s	518.87	Joback Method
dvisc	0.0001297	Pa×s	569.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64863e+01
Coeff. B	-5.36578e+03
Coeff. C	-9.68720e+01
Temperature range (K), min.	428.12
Temperature range (K), max.	577.04

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R89427&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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume