Hexadecene

Inchi: InChI=1S/C16H32/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3H,1,4-16H2,2H3
InchiKey: GQEZCXVZFLOKMC-UHFFFAOYSA-N
Formula: C16H32
SMILES: C=CCCCCCCCCCCCCCC
Mol. weight [g/mol]: 224.43
CAS: 26952-14-7

Physical Properties

Property code	Value	Unit	Source
gf	171.68	kJ/mol	Joback Method
hf	-248.14	kJ/mol	Joback Method
hfus	35.92	kJ/mol	Joback Method
hvap	50.54	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.264		Crippen Method
mcvol	232.000	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1592.00		NIST Webbook
ripol	1630.00		NIST Webbook
tb	562.16	K	Joback Method
tc	723.12	K	Joback Method
tf	268.32	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.88	J/mol×K	562.16	Joback Method
cpg	609.62	J/mol×K	588.99	Joback Method
cpg	627.60	J/mol×K	615.81	Joback Method
cpg	644.86	J/mol×K	642.64	Joback Method

cpg	661.40	J/mol×K	669.47	Joback Method
cpg	677.27	J/mol×K	696.30	Joback Method
cpg	692.47	J/mol×K	723.12	Joback Method
dvisc	0.0047648	Pa×s	268.32	Joback Method
dvisc	0.0017394	Pa×s	317.29	Joback Method
dvisc	0.0008313	Pa×s	366.27	Joback Method
dvisc	0.0004729	Pa×s	415.24	Joback Method
dvisc	0.0003030	Pa×s	464.21	Joback Method
dvisc	0.0002114	Pa×s	513.19	Joback Method
dvisc	0.0001570	Pa×s	562.16	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26952147&Units=SI

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
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