Hexadecane, 1-iodo-

Other names:	1-Iodohexadecane
	Cetyl iodide
	Hexadecyl iodide
	n-Hexadecyl iodide
Inchi:	InChI=1S/C16H33I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h2-16H2,1H3
InchiKey:	KMWHQYDMBYABKL-UHFFFAOYSA-N
Formula:	C16H33I
SMILES:	CCCCCCCCCCCCCCCCI
Mol. weight [g/mol]:	352.34
CAS:	544-77-4

Physical Properties

Property code	Value	Unit	Source
gf	141.96	kJ/mol	Joback Method
hf	-296.70	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	99.60	kJ/mol	NIST Webbook
log10ws	-7.47		Crippen Method
logp	6.903		Crippen Method
mcvol	262.120	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2038.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2064.00		NIST Webbook
ripol	2362.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	658.62	K	Joback Method
tc	838.91	K	Joback Method
tf	293.00 ± 3.00	K	NIST Webbook
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.39	J/mol×K	658.62	Joback Method
cpg	707.74	J/mol×K	688.67	Joback Method
cpg	725.24	J/mol×K	718.72	Joback Method
cpg	741.92	J/mol×K	748.77	Joback Method
cpg	757.80	J/mol×K	778.82	Joback Method
cpg	772.94	J/mol×K	808.86	Joback Method
cpg	787.36	J/mol×K	838.91	Joback Method
dvisc	0.0035352	Pa×s	328.14	Joback Method
dvisc	0.0013651	Pa×s	383.22	Joback Method
dvisc	0.0006695	Pa×s	438.30	Joback Method
dvisc	0.0003850	Pa×s	493.38	Joback Method
dvisc	0.0002474	Pa×s	548.46	Joback Method
dvisc	0.0001724	Pa×s	603.54	Joback Method
dvisc	0.0001276	Pa×s	658.62	Joback Method
hvapt	73.00	kJ/mol	574.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	479.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64627e+01
Coeff. B	-5.86815e+03
Coeff. C	-1.16332e+02
Temperature range (K), min.	479.12
Temperature range (K), max.	642.56

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544774&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume