Eicosane, 1-iodo-

Other names: 1-Iodoeicosane
Inchi: InChI=1S/C20H41I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h2-20H2,1
InchiKey: UYBWORFIJZQKEP-UHFFFAOYSA-N
Formula: C20H41I
SMILES: CCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 408.44
CAS: 34994-81-5

Physical Properties

Property code	Value	Unit	Source
gf	175.64	kJ/mol	Joback Method
hf	-379.26	kJ/mol	Joback Method
hfus	51.96	kJ/mol	Joback Method
hvap	118.50	kJ/mol	NIST Webbook
log10ws	-9.14		Crippen Method
logp	8.463		Crippen Method
mcvol	318.480	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
tb	750.14	K	Joback Method
tc	930.35	K	Joback Method
tf	314.60 ± 1.50	K	NIST Webbook
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.09	J/mol×K	930.35	Joback Method
cpg	1011.59	J/mol×K	900.31	Joback Method
cpg	995.33	J/mol×K	870.28	Joback Method
cpg	978.25	J/mol×K	840.24	Joback Method
cpg	960.32	J/mol×K	810.21	Joback Method
cpg	941.49	J/mol×K	780.17	Joback Method

cpg	921.72	J/mol×K	750.14	Joback Method
dvisc	0.0022797	Pa×s	373.22	Joback Method
dvisc	0.0000737	Pa×s	750.14	Joback Method
dvisc	0.0001005	Pa×s	687.32	Joback Method
dvisc	0.0001460	Pa×s	624.50	Joback Method
dvisc	0.0002305	Pa×s	561.68	Joback Method
dvisc	0.0004082	Pa×s	498.86	Joback Method
dvisc	0.0008522	Pa×s	436.04	Joback Method
hvapt	80.90	kJ/mol	594.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62087e+01
Coeff. B	-6.19153e+03
Coeff. C	-1.30232e+02
Temperature range (K), min.	519.12
Temperature range (K), max.	698.41

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34994815&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume