

Tridecane, 1-iodo-

Other names:	1-Iodotridecane Tridecyl iodide
Inchi:	InChI=1S/C13H27I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h2-13H2,1H3
InchiKey:	XGAMQNYEIPCUIZ-UHFFFAOYSA-N
Formula:	C13H27I
SMILES:	CCCCCCCCCCCCCI
Mol. weight [g/mol]:	310.26
CAS:	35599-77-0

Physical Properties

Property code	Value	Unit	Source
gf	116.70	kJ/mol	Joback Method
hf	-234.78	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	85.00	kJ/mol	NIST Webbook
log10ws	-6.21		Crippen Method
logp	5.732		Crippen Method
mcvol	219.850	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	589.98	K	Joback Method
tc	774.58	K	Joback Method
tf	294.33	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.91	J/mol×K	774.58	Joback Method
cpg	605.56	J/mol×K	743.82	Joback Method
cpg	591.55	J/mol×K	713.05	Joback Method
cpg	576.82	J/mol×K	682.28	Joback Method
cpg	561.36	J/mol×K	651.51	Joback Method
cpg	545.13	J/mol×K	620.75	Joback Method
cpg	528.10	J/mol×K	589.98	Joback Method

dvisc	0.0046336	Pa×s	294.33	Joback Method
dvisc	0.0001856	Pa×s	589.98	Joback Method
dvisc	0.0002485	Pa×s	540.71	Joback Method
dvisc	0.0003527	Pa×s	491.43	Joback Method
dvisc	0.0005415	Pa×s	442.16	Joback Method
dvisc	0.0009256	Pa×s	392.88	Joback Method
dvisc	0.0018450	Pa×s	343.61	Joback Method
hvapt	66.10	kJ/mol	547.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.65477e+01
Coeff. B	-5.53401e+03
Coeff. C	-1.04378e+02
Temperature range (K), min.	444.72
Temperature range (K), max.	596.89

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=C35599770&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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