

Triacontane, 1-iodo-

Inchi: InChI=1S/C30H61I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30
InchiKey: WPPHWXZEMRXEHC-UHFFFAOYSA-N
Formula: C30H61I
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 548.71

Physical Properties

Property code	Value	Unit	Source
gf	259.84	kJ/mol	Joback Method
hf	-585.66	kJ/mol	Joback Method
hfus	77.86	kJ/mol	Joback Method
hvap	91.75	kJ/mol	Joback Method
log10ws	-13.33		Crippen Method
logp	12.364		Crippen Method
mvol	459.380	ml/mol	McGowan Method
pc	589.12	kPa	Joback Method
rinpol	3559.00		NIST Webbook
rinpol	3559.00		NIST Webbook
tb	978.94	K	Joback Method
tc	1209.58	K	Joback Method
tf	485.92	K	Joback Method
vc	1.804	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.86	J/molxK	978.94	Joback Method
cpg	1587.73	J/molxK	1017.38	Joback Method
cpg	1612.08	J/molxK	1055.82	Joback Method
cpg	1635.04	J/molxK	1094.26	Joback Method
cpg	1656.76	J/molxK	1132.70	Joback Method
cpg	1677.35	J/molxK	1171.14	Joback Method
cpg	1696.96	J/molxK	1209.58	Joback Method
dvisc	0.0005963	Paxs	485.92	Joback Method

dvisc	0.0002110	Paxs	568.09	Joback Method
dvisc	0.0000970	Paxs	650.26	Joback Method
dvisc	0.0000531	Paxs	732.43	Joback Method
dvisc	0.0000329	Paxs	814.60	Joback Method
dvisc	0.0000222	Paxs	896.77	Joback Method
dvisc	0.0000160	Paxs	978.94	Joback Method

Sources

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=U406323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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