triacontane, 1-iodo-

Inchi: InChI=1S/C30H61I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: WPPHWXZEMRXEHC-UHFFFAOYSA-N
Formula: C30H61I
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 548.71
CAS: 62154-82-9

Physical Properties

Property code	Value	Unit	Source
af	1.2500		Cheméo Relay (1.0)
gf	259.84	kJ/mol	Joback Method
hf	-610.65	kJ/mol	Cheméo Relay (1.0)
hfus	77.86	kJ/mol	Joback Method
hvap	166.49	kJ/mol	Cheméo Relay (1.0)
ie	9.81	eV	Cheméo Relay (1.0)
log10ws	-11.61		Cheméo Relay (1.0)
logp	12.364		Crippen Method
mcvol	459.380	ml/mol	McGowan Method
pc	589.12	kPa	Joback Method
tb	685.60	K	Cheméo Relay (1.0)
tc	870.06	K	Cheméo Relay (1.0)
tf	336.74	K	Cheméo Relay (1.0)
vc	1.801	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0000531	Pa×s	732.43	Joback Method
dvisc	0.0000160	Pa×s	978.94	Joback Method
dvisc	0.0000222	Pa×s	896.77	Joback Method
dvisc	0.0000329	Pa×s	814.60	Joback Method
dvisc	0.0005963	Pa×s	485.92	Joback Method
dvisc	0.0000970	Pa×s	650.26	Joback Method
dvisc	0.0002110	Pa×s	568.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62154829&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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