dotriacontane, 1-iodo-

Inchi: InChI=1S/C32H65I/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: JXFRLKULJKAXNM-UHFFFAOYSA-N
Formula: C32H65I
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 576.76
CAS: 62154-83-0

Physical Properties

Property code	Value	Unit	Source
af	1.3202		Cheméo Relay (1.0)
gf	276.68	kJ/mol	Joback Method
hf	-651.94	kJ/mol	Cheméo Relay (1.0)
hfus	83.04	kJ/mol	Joback Method
hvap	176.03	kJ/mol	Cheméo Relay (1.0)
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-12.16		Cheméo Relay (1.0)
logp	13.144		Crippen Method
mcvol	487.560	ml/mol	McGowan Method
pc	537.83	kPa	Joback Method
tb	697.92	K	Cheméo Relay (1.0)
tc	881.13	K	Cheméo Relay (1.0)
tf	339.88	K	Cheméo Relay (1.0)
vc	1.910	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1696.72	J/mol×K	1024.70	Joback Method
cpg	1724.87	J/mol×K	1067.03	Joback Method
cpg	1751.28	J/mol×K	1109.37	Joback Method
cpg	1776.12	J/mol×K	1151.70	Joback Method
cpg	1799.59	J/mol×K	1194.04	Joback Method
cpg	1821.87	J/mol×K	1236.37	Joback Method
cpg	1843.15	J/mol×K	1278.71	Joback Method

dvisc	0.0004434	Pa×s	508.46	Joback Method
dvisc	0.0001556	Pa×s	594.50	Joback Method
dvisc	0.0000712	Pa×s	680.54	Joback Method
dvisc	0.0000388	Pa×s	766.58	Joback Method
dvisc	0.0000239	Pa×s	852.62	Joback Method
dvisc	0.0000161	Pa×s	938.66	Joback Method
dvisc	0.0000116	Pa×s	1024.70	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=C62154830&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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