hexacosane, 1-iodo-

Inchi: InChI=1S/C26H53I/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: QLWJHYYRERTPQW-UHFFFAOYSA-N
Formula: C26H53I
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 492.60
CAS: 52644-81-2

Physical Properties

Property code	Value	Unit	Source
af	1.1095		Cheméo Relay (1.0)
gf	226.16	kJ/mol	Joback Method
hf	-527.71	kJ/mol	Cheméo Relay (1.0)
hfus	67.50	kJ/mol	Joback Method
hvap	147.31	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-10.52		Cheméo Relay (1.0)
logp	10.804		Crippen Method
mcvol	403.020	ml/mol	McGowan Method
pc	716.45	kPa	Joback Method
tb	660.96	K	Cheméo Relay (1.0)
tc	847.10	K	Cheméo Relay (1.0)
tf	329.68	K	Cheméo Relay (1.0)
vc	1.582	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.93	J/mol×K	887.42	Joback Method
cpg	1320.52	J/mol×K	920.62	Joback Method
cpg	1341.92	J/mol×K	953.82	Joback Method
cpg	1362.22	J/mol×K	987.01	Joback Method
cpg	1381.47	J/mol×K	1020.21	Joback Method
cpg	1399.76	J/mol×K	1053.41	Joback Method
cpg	1417.15	J/mol×K	1086.61	Joback Method

dvisc	0.0010527	Pa×s	440.84	Joback Method
dvisc	0.0003794	Pa×s	515.27	Joback Method
dvisc	0.0001770	Pa×s	589.70	Joback Method
dvisc	0.0000979	Pa×s	664.13	Joback Method
dvisc	0.0000610	Pa×s	738.56	Joback Method
dvisc	0.0000415	Pa×s	812.99	Joback Method
dvisc	0.0000301	Pa×s	887.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C52644812&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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