

Hexacosane, 1-iodo-

Inchi:	InChI=1S/C26H53I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	QLWJHYRERTPQW-UHFFFAOYSA-N
Formula:	C26H53I
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]:	492.60

Physical Properties

Property code	Value	Unit	Source
gf	226.16	kJ/mol	Joback Method
hf	-503.10	kJ/mol	Joback Method
hfus	67.50	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-11.65		Crippen Method
logp	10.804		Crippen Method
mcvol	403.020	ml/mol	McGowan Method
pc	716.45	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	887.42	K	Joback Method
tc	1086.61	K	Joback Method
tf	440.84	K	Joback Method
vc	1.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.93	J/molxK	887.42	Joback Method
cpg	1399.76	J/molxK	1053.41	Joback Method
cpg	1381.47	J/molxK	1020.21	Joback Method
cpg	1362.22	J/molxK	987.01	Joback Method
cpg	1341.92	J/molxK	953.82	Joback Method
cpg	1320.52	J/molxK	920.62	Joback Method
cpg	1417.15	J/molxK	1086.61	Joback Method
dvisc	0.0000301	Paxs	887.42	Joback Method

dvisc	0.0000415	Paxs	812.99	Joback Method
dvisc	0.0000610	Paxs	738.56	Joback Method
dvisc	0.0000979	Paxs	664.13	Joback Method
dvisc	0.0001770	Paxs	589.70	Joback Method
dvisc	0.0003794	Paxs	515.27	Joback Method
dvisc	0.0010527	Paxs	440.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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