Perfluorohexyl iodide

Other names:	Perfluoro-n-hexyl iodide
	1-Iodoperfluorohexane
	Tridecafluorohexyl iodide
	Hexane, 1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodo-
	1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodohexane
Inchi:	InChI=1S/C6F13I/c7-1(8,3(11,12)5(15,16)17)2(9,10)4(13,14)6(18,19)20
InchiKey:	BULLJMKUVKYZDJ-UHFFFAOYSA-N
Formula:	C6F13I
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I
Mol. weight [g/mol]:	445.95
CAS:	355-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-2457.73	kJ/mol	Joback Method
hf	-2692.23	kJ/mol	Joback Method
hfus	11.26	kJ/mol	Joback Method
hvap	19.93	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.118		Crippen Method
mcvol	144.230	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	400.95	K	Joback Method
tc	547.74	K	Joback Method
tf	237.63	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.55	J/mol×K	400.95	Joback Method
cpg	340.42	J/mol×K	425.41	Joback Method
cpg	351.27	J/mol×K	449.88	Joback Method
cpg	361.14	J/mol×K	474.34	Joback Method

cpg	370.09	J/mol×K	498.81	Joback Method
cpg	378.18	J/mol×K	523.27	Joback Method
cpg	385.46	J/mol×K	547.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.50 ± 0.50	K	11.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C355431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/38-308-8/Perfluorohexyl-iodide.pdf

Generated by Cheméo on 2024-10-12 04:13:27.663754768 +0000 UTC m=+3287270.300724016.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.