TRIDECAFLUOROHEXYL 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]:	445.94

Physical Properties

Property code	Value	Unit	Source
af	0.4526		Cheméo Relay (1.0)
gf	-2457.73	kJ/mol	Joback Method
hf	-2696.93	kJ/mol	Cheméo Relay (1.0)
hfus	11.26	kJ/mol	Joback Method
hvap	43.29	kJ/mol	Cheméo Relay (1.0)
ie	10.29	eV	Cheméo Relay (1.0)
logp	5.118		Crippen Method
mcvol	144.230	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	385.94	K	Cheméo Relay (1.0)
tc	526.14	K	Cheméo Relay (1.0)
tf	215.16	K	Cheméo Relay (1.0)
vc	0.603	m3/kmol	Cheméo Relay (1.0)

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C355431&Units=SI

Legend

af: Acentric Factor
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
ie: Ionization energy
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