1,6-Diiododecafluorohexane

Other names: 1,6-diiodoperfluorohexane
Inchi: InChI=1S/C6F12I2/c7-1(8,3(11,12)5(15,16)19)2(9,10)4(13,14)6(17,18)20
InchiKey: JOQDDLBOAIKFQX-UHFFFAOYSA-N
Formula: C6F12I2
SMILES: FC(F)(I)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I
Mol. weight [g/mol]: 553.85
CAS: 375-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-2204.80	kJ/mol	Joback Method
hf	-2419.25	kJ/mol	Joback Method
hfus	12.58	kJ/mol	Joback Method
hvap	30.12	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	5.583		Crippen Method
mcvol	168.280	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1019.00		NIST Webbook
tb	494.82	K	Joback Method
tc	678.31	K	Joback Method
tf	295.10	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.99	J/mol×K	494.82	Joback Method
cpg	385.77	J/mol×K	525.40	Joback Method
cpg	394.26	J/mol×K	555.98	Joback Method
cpg	401.58	J/mol×K	586.57	Joback Method

cpg	407.83	J/mol×K	617.15	Joback Method
cpg	413.13	J/mol×K	647.73	Joback Method
cpg	417.58	J/mol×K	678.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.00	K	13.30	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume