

Perfluorodecyl iodide

Other names:	1-Iodoperfluorodecane Decane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoro-10-iodo-henicosafuoro-10-iododecane
Inchi:	InChI=1S/C10F21I/c11-1(12,3(15,16)5(19,20)7(23,24)9(27,28)29)2(13,14)4(17,18)6(21,22)10
InchiKey:	UDWBMXSQHOHKOI-UHFFFAOYSA-N
Formula:	C10F21I
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I
Mol. weight [g/mol]:	645.98
CAS:	423-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-3971.17	kJ/mol	Joback Method
hf	-4378.67	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	17.11	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.659		Crippen Method
mcvol	214.750	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
tb	470.50 ± 2.50	K	NIST Webbook
tc	602.71	K	Joback Method
tf	297.11	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.11	J/mol×K	473.71	Joback Method
cpg	592.24	J/mol×K	495.21	Joback Method
cpg	604.25	J/mol×K	516.71	Joback Method
cpg	615.22	J/mol×K	538.21	Joback Method
cpg	625.19	J/mol×K	559.71	Joback Method
cpg	634.22	J/mol×K	581.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C423621&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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