

1,10-Diiodoperfluorodecane

Inchi:	InChI=1S/C10F20I2/c11-1(12,3(15,16)5(19,20)7(23,24)9(27,28)31)2(13,14)4(17,18)6(21,
InchiKey:	QBEWJJSQJWLVAI-UHFFFAOYSA-N
Formula:	C10F20I2
SMILES:	FC(F)(I)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)C(F)(F)I
Mol. weight [g/mol]:	753.88

Physical Properties

Property code	Value	Unit	Source
gf	-3718.24	kJ/mol	Joback Method
hf	-4105.69	kJ/mol	Joback Method
hfus	17.93	kJ/mol	Joback Method
hvap	27.30	kJ/mol	Joback Method
log10ws	-10.03		Crippen Method
logp	8.124		Crippen Method
mcvol	238.800	ml/mol	McGowan Method
pc	1163.25	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1243.00		NIST Webbook
tb	567.58	K	Joback Method
tc	723.55	K	Joback Method
tf	354.58	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.97	J/mol×K	567.58	Joback Method
cpg	645.03	J/mol×K	593.57	Joback Method
cpg	653.86	J/mol×K	619.57	Joback Method
cpg	661.56	J/mol×K	645.56	Joback Method
cpg	668.24	J/mol×K	671.56	Joback Method
cpg	674.00	J/mol×K	697.55	Joback Method
cpg	678.96	J/mol×K	723.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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