

Difluorodinitromethane

Inchi: InChI=1S/CF2N2O4/c2-1(3,4(6)7)5(8)9
InchiKey: PLHQSNLSBKPCTC-UHFFFAOYSA-N
Formula: CF2N2O4
SMILES: O=[N+]([O-])C(F)(F)[N+](=O)[O-]
Mol. weight [g/mol]: 142.02
CAS: 1185-11-1

Physical Properties

Property code	Value	Unit	Source
chl	-307.00 ± 5.90	kJ/mol	NIST Webbook
gf	-358.14	kJ/mol	Joback Method
hf	-403.00 ± 6.70	kJ/mol	NIST Webbook
hfl	-444.80 ± 6.70	kJ/mol	NIST Webbook
hfus	19.81	kJ/mol	Joback Method
hvap	41.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-1.71		Crippen Method
logp	0.090		Crippen Method
mcvol	63.330	ml/mol	McGowan Method
pc	5398.63	kPa	Joback Method
tb	521.27	K	Joback Method
tc	763.54	K	Joback Method
tf	391.85	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.53	J/molxK	723.16	Joback Method
cpg	144.60	J/molxK	521.27	Joback Method
cpg	149.89	J/molxK	561.65	Joback Method
cpg	154.58	J/molxK	602.03	Joback Method
cpg	158.72	J/molxK	642.40	Joback Method
cpg	162.35	J/molxK	682.78	Joback Method
cpg	168.31	J/molxK	763.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1185111&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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