1,8-Difluoro-1,1,3,6,8,8-hexanitro-3,6-diazaoctane

Inchi: InChI=1S/C6H8F2N8O12/c7-5(11(17)18,12(19)20)3-9(15(25)26)1-2-10(16(27)28)4-6(8,1
InchiKey: CEKYSAGUWBZXMH-UHFFFAOYSA-N
Formula: C6H8F2N8O12
SMILES: O=[N+]([O-])N(CCN(CC(F)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])CC(F)([N+](=O)[O-])[N
Mol. weight [g/mol]: 422.17
CAS: 28820-56-6

Physical Properties

Property code	Value	Unit	Source
chs	-3335.20 ± 4.60	kJ/mol	NIST Webbook
gf	50.56	kJ/mol	Joback Method
hf	-506.39	kJ/mol	Joback Method
hfs	-527.80 ± 4.60	kJ/mol	NIST Webbook
hfus	76.84	kJ/mol	Joback Method
hvap	128.36	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	-1.673		Crippen Method
mcvol	223.420	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	1264.68	K	Joback Method
tc	1559.15	K	Joback Method
tf	1090.00	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.63	J/mol×K	1264.68	Joback Method
cpg	750.82	J/mol×K	1313.76	Joback Method
cpg	761.15	J/mol×K	1362.84	Joback Method
cpg	772.91	J/mol×K	1411.91	Joback Method
cpg	786.39	J/mol×K	1460.99	Joback Method
cpg	801.88	J/mol×K	1510.07	Joback Method
cpg	819.67	J/mol×K	1559.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28820566&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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