

1,8-Difluoro-3-oxa-5-aza-1,1,5,8,8-pentanitrooctan

Inchi:	InChI=1S/C6H8F2N6O11/c7-5(10(15)16,11(17)18)2-1-3-9(14(23)24)4-25-6(8,12(19)20)1
InchiKey:	XXYVHYYYUJTAME-UHFFFAOYSA-N
Formula:	C6H8F2N6O11
SMILES:	O=[N+]([O-])N(CCCC(F)([N+](=O)[O-])[N+](=O)[O-])COC(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	378.16
CAS:	80308-84-5

Physical Properties

Property code	Value	Unit	Source
chs	-3136.30 ± 0.80	kJ/mol	NIST Webbook
chs	-3136.30 ± 1.30	kJ/mol	NIST Webbook
gf	-200.77	kJ/mol	Joback Method
hf	-695.38	kJ/mol	Joback Method
hfs	-727.20 ± 1.30	kJ/mol	NIST Webbook
hfs	-727.20 ± 1.30	kJ/mol	NIST Webbook
hfus	63.64	kJ/mol	Joback Method
hvap	112.13	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	-0.455		Crippen Method
mcvol	201.890	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	1122.82	K	Joback Method
tc	1398.94	K	Joback Method
tf	936.15	K	Joback Method
vc	0.832	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.07	J/mol×K	1122.82	Joback Method
cpg	655.48	J/mol×K	1168.84	Joback Method
cpg	660.76	J/mol×K	1214.86	Joback Method
cpg	666.08	J/mol×K	1260.88	Joback Method
cpg	671.61	J/mol×K	1306.90	Joback Method

cpg	677.53	J/mol×K	1352.92	Joback Method
cpg	684.00	J/mol×K	1398.94	Joback Method

Sources

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=C80308845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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