1,1'-Oxybis(2,4,4-trinitro-4-fluoro-2-azabutane)

Inchi: InChI=1S/C6H8F2N8O13/c7-5(11(17)18,12(19)20)1-9(15(25)26)3-29-4-10(16(27)28)2-6(
InchiKey: QGCZQMUQUNUTBO-UHFFFAOYSA-N
Formula: C6H8F2N8O13
SMILES: O=[N+]([O-])N(COCN(CC(F)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])CC(F)([N+](=O)[O-]
Mol. weight [g/mol]: 438.17
CAS: 29414-46-8

Physical Properties

Property code	Value	Unit	Source
chs	-3199.10 ± 3.30	kJ/mol	NIST Webbook
gf	-54.44	kJ/mol	Joback Method
hf	-638.61	kJ/mol	Joback Method
hfs	-664.40 ± 3.30	kJ/mol	NIST Webbook
hfus	78.02	kJ/mol	Joback Method
hvap	130.77	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	-1.741		Crippen Method
mcvol	229.290	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	1287.10	K	Joback Method
tc	1582.40	K	Joback Method
tf	1112.23	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.90	J/mol×K	1287.10	Joback Method
cpg	763.90	J/mol×K	1336.32	Joback Method
cpg	771.66	J/mol×K	1385.53	Joback Method
cpg	780.42	J/mol×K	1434.75	Joback Method
cpg	790.44	J/mol×K	1483.97	Joback Method
cpg	801.98	J/mol×K	1533.18	Joback Method
cpg	815.28	J/mol×K	1582.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29414468&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