Difluoro-bis(2-fluoro-2,2-dinitroethoxy)methane

Inchi: InChI=1S/C5H4F4N4O10/c6-3(10(14)15,11(16)17)1-22-5(8,9)23-2-4(7,12(18)19)13(20)2
InchiKey: ZRXYSSKJEJXCDB-UHFFFAOYSA-N
Formula: C5H4F4N4O10
SMILES: O=[N+]([O-])C(F)(COC(F)(F)OCC(F)([N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 356.10
CAS: 58715-08-5

Physical Properties

Property code	Value	Unit	Source
chl	-1982.90 ± 6.70	kJ/mol	NIST Webbook
gf	-847.30	kJ/mol	Joback Method
hf	-1264.70	kJ/mol	Joback Method
hfl	-1297.90 ± 6.70	kJ/mol	NIST Webbook
hfus	46.60	kJ/mol	Joback Method
hvap	90.75	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	-0.077		Crippen Method
mcvol	169.810	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	953.39	K	Joback Method
tc	1210.98	K	Joback Method
tf	774.63	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.83	J/mol×K	953.39	Joback Method
cpg	531.52	J/mol×K	996.32	Joback Method
cpg	535.63	J/mol×K	1039.25	Joback Method
cpg	539.29	J/mol×K	1082.18	Joback Method
cpg	542.62	J/mol×K	1125.11	Joback Method
cpg	545.74	J/mol×K	1168.04	Joback Method
cpg	548.77	J/mol×K	1210.98	Joback Method

hvapt	72.70	kJ/mol	340.00	NIST Webbook

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=C58715085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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