N,N'-Bis(2-fluoro-2,2-dinitroethyl)ethanediamide

Inchi: InChI=1S/C6H6F2N6O10/c7-5(11(17)18,12(19)20)1-9-3(15)4(16)10-2-6(8,13(21)22)14(2
InchiKey: SWUZCYNGXFKYCY-UHFFFAOYSA-N
Formula: C6H6F2N6O10
SMILES: O=C(NCC(F)([N+](=O)[O-])[N+](=O)[O-])C(=O)NCC(F)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 360.14
CAS: 40488-97-9

Physical Properties

Property code	Value	Unit	Source
chs	-2599.50 ± 3.40	kJ/mol	NIST Webbook
gf	-321.16	kJ/mol	Joback Method
hf	-738.15	kJ/mol	Joback Method
hfs	-977.90 ± 6.90	kJ/mol	NIST Webbook
hfus	61.47	kJ/mol	Joback Method
hvap	117.45	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	-2.428		Crippen Method
mcvol	191.720	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	1144.20	K	Joback Method
tc	1417.94	K	Joback Method
tf	943.02	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.99	J/mol×K	1144.20	Joback Method
cpg	603.62	J/mol×K	1189.82	Joback Method
cpg	608.29	J/mol×K	1235.45	Joback Method
cpg	613.16	J/mol×K	1281.07	Joback Method
cpg	618.41	J/mol×K	1326.69	Joback Method
cpg	624.20	J/mol×K	1372.32	Joback Method
cpg	630.70	J/mol×K	1417.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40488979&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

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