2',4'-Dinitro-5'-fluoroacetanilide

Inchi: InChI=1S/C8H6FN3O5/c1-4(13)10-6-2-5(9)7(11(14)15)3-8(6)12(16)17/h2-3H,1H3,(H,10,
InchiKey: LZBXUWOTXPNTNQ-UHFFFAOYSA-N
Formula: C8H6FN3O5
SMILES: CC(=O)Nc1cc(F)c([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 243.15
CAS: 1548-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-63.24	kJ/mol	Joback Method
hf	-283.07	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	83.21	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	1.601		Crippen Method
mcvol	147.980	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
tb	831.05	K	Joback Method
tc	1087.11	K	Joback Method
tf	634.30	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.41	J/mol×K	831.05	Joback Method
cpg	411.30	J/mol×K	873.73	Joback Method
cpg	418.34	J/mol×K	916.40	Joback Method
cpg	424.58	J/mol×K	959.08	Joback Method
cpg	430.06	J/mol×K	1001.76	Joback Method
cpg	434.81	J/mol×K	1044.43	Joback Method
cpg	438.87	J/mol×K	1087.11	Joback Method

Sources

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=C1548181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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