Glutamic acid, n-(2,5-difluoro-4-nitrobenzoyl)-

Inchi: InChI=1S/C12H10F2N2O7/c13-6-4-9(16(22)23)7(14)3-5(6)11(19)15-8(12(20)21)1-2-10(1

InchiKey: SVQAWECNXJIAHF-UHFFFAOYSA-N

Formula: C12H10F2N2O7

SMILES: O=C(O)CCC(NC(=O)c1cc(F)c([N+](=O)[O-])cc1F)C(=O)O

Mol. weight [g/mol]: 332.21

Physical Properties

Property code	Value	Unit	Source
gf	-793.84	kJ/mol	Joback Method
hf	-1085.88	kJ/mol	Joback Method
hfus	51.78	kJ/mol	Joback Method
hvap	121.17	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	0.921		Crippen Method
mcvol	203.570	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	1061.66	K	Joback Method
tc	1299.78	K	Joback Method
tf	742.86	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.39	J/mol×K	1061.66	Joback Method
cpg	627.41	J/mol×K	1101.35	Joback Method
cpg	631.66	J/mol×K	1141.03	Joback Method
cpg	635.18	J/mol×K	1180.72	Joback Method
cpg	638.02	J/mol×K	1220.41	Joback Method
cpg	640.22	J/mol×K	1260.10	Joback Method
cpg	641.83	J/mol×K	1299.78	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=B6008662&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