Benzoic acid, 2,5-difluoro-4-nitro

Inchi: InChI=1S/C7H3F2NO4/c8-4-2-6(10(13)14)5(9)1-3(4)7(11)12/h1-2H,(H,11,12)
InchiKey: GPTNSBLYGCZJQV-UHFFFAOYSA-N
Formula: C7H3F2NO4
SMILES: O=C(O)c1cc(F)c([N+](=O)[O-])cc1F
Mol. weight [g/mol]: 203.10
CAS: 116465-48-6

Physical Properties

Property code	Value	Unit	Source
gf	-528.23	kJ/mol	Joback Method
hf	-653.48	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	1.571		Crippen Method
mcvol	114.130	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	697.61	K	Joback Method
tc	913.71	K	Joback Method
tf	488.17	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.50	J/mol×K	697.61	Joback Method
cpg	287.01	J/mol×K	733.63	Joback Method
cpg	293.03	J/mol×K	769.64	Joback Method
cpg	298.57	J/mol×K	805.66	Joback Method
cpg	303.64	J/mol×K	841.68	Joback Method
cpg	308.28	J/mol×K	877.69	Joback Method
cpg	312.48	J/mol×K	913.71	Joback Method

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=C116465486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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