Benzamide, N-(3-nitrophenyl)-3-fluoro-

Inchi: InChI=1S/C13H9FN2O3/c14-10-4-1-3-9(7-10)13(17)15-11-5-2-6-12(8-11)16(18)19/h1-8H
InchiKey: UIIRKXRFILYYBR-UHFFFAOYSA-N
Formula: C13H9FN2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1cccc(F)c1
Mol. weight [g/mol]: 260.22

Physical Properties

Property code	Value	Unit	Source
gf	65.35	kJ/mol	Joback Method
hf	-127.51	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	2.986		Crippen Method
mcvol	177.250	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	2375.00		NIST Webbook
tb	815.31	K	Joback Method
tc	1072.15	K	Joback Method
tf	560.94	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.30	J/mol×K	815.31	Joback Method
cpg	497.98	J/mol×K	858.12	Joback Method
cpg	507.58	J/mol×K	900.92	Joback Method
cpg	516.17	J/mol×K	943.73	Joback Method
cpg	523.85	J/mol×K	986.53	Joback Method
cpg	530.69	J/mol×K	1029.34	Joback Method
cpg	536.77	J/mol×K	1072.15	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=U307169&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume