Benzamide, N-(3-nitrophenyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C13H7F3N2O3/c14-10-5-4-9(11(15)12(10)16)13(19)17-7-2-1-3-8(6-7)18(20)21
InchiKey: ATLXDZIKDUZLIH-UHFFFAOYSA-N
Formula: C13H7F3N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 296.20

Physical Properties

Property code	Value	Unit	Source
gf	-343.53	kJ/mol	Joback Method
hf	-542.67	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	79.05	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.264		Crippen Method
mcvol	180.790	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	2237.00		NIST Webbook
tb	823.81	K	Joback Method
tc	1062.16	K	Joback Method
tf	587.16	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.86	J/mol×K	823.81	Joback Method
cpg	508.32	J/mol×K	863.54	Joback Method
cpg	516.87	J/mol×K	903.26	Joback Method
cpg	524.55	J/mol×K	942.99	Joback Method
cpg	531.41	J/mol×K	982.71	Joback Method
cpg	537.50	J/mol×K	1022.44	Joback Method
cpg	542.88	J/mol×K	1062.16	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=U307180&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume