2,3,4,5,6-Pentafluoro-N-(3-nitrophenyl)benzamide

Other names: Benzamide, N-(3-nitrophenyl)-2,3,4,5,6-pentafluoro-
Inchi: InChI=1S/C13H5F5N2O3/c14-8-7(9(15)11(17)12(18)10(8)16)13(21)19-5-2-1-3-6(4-5)20(
InchiKey: AAYFOOIDAKNNRI-UHFFFAOYSA-N
Formula: C13H5F5N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 332.18
CAS: 304444-14-2

Physical Properties

Property code	Value	Unit	Source
gf	-752.41	kJ/mol	Joback Method
hf	-957.83	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	78.74	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	3.543		Crippen Method
mcvol	184.330	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	2169.00		NIST Webbook
tb	832.31	K	Joback Method
tc	1055.72	K	Joback Method
tf	613.38	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.24	J/mol×K	832.31	Joback Method
cpg	518.70	J/mol×K	869.55	Joback Method
cpg	526.35	J/mol×K	906.78	Joback Method
cpg	533.24	J/mol×K	944.02	Joback Method
cpg	539.39	J/mol×K	981.25	Joback Method
cpg	544.82	J/mol×K	1018.49	Joback Method
cpg	549.58	J/mol×K	1055.72	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=C304444142&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