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

Inchi: InChI=1S/C14H9F3N2O3/c15-14(16,17)10-4-1-3-9(7-10)13(20)18-11-5-2-6-12(8-11)19(2

InchiKey: MEYXYYXOUMOXSA-UHFFFAOYSA-N

Formula: C14H9F3N2O3

SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 310.23

Physical Properties

Property code	Value	Unit	Source
gf	-313.01	kJ/mol	Joback Method
hf	-549.12	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.866		Crippen Method
mcvol	194.880	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	2372.00		NIST Webbook
tb	833.50	K	Joback Method
tc	1077.80	K	Joback Method
tf	575.81	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.56	J/mol×K	833.50	Joback Method
cpg	567.70	J/mol×K	874.22	Joback Method
cpg	576.86	J/mol×K	914.93	Joback Method
cpg	585.14	J/mol×K	955.65	Joback Method
cpg	592.65	J/mol×K	996.37	Joback Method
cpg	599.51	J/mol×K	1037.08	Joback Method
cpg	605.81	J/mol×K	1077.80	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=U306940&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