3,5-Bis(trifluoromethyl)benzamide

Other names: 3,5-di(Trifluoromethyl)benzamide
Benzamide, 3,5-bis(trifluoromethyl)-
Inchi: InChI=1S/C9H5F6NO/c10-8(11,12)5-1-4(7(16)17)2-6(3-5)9(13,14)15/h1-3H,(H2,16,17)
InchiKey: YNOPIKHMZIOWHS-UHFFFAOYSA-N
Formula: C9H5F6NO
SMILES: NC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 257.13
CAS: 22227-26-5

Physical Properties

Property code	Value	Unit	Source
gf	-1107.60	kJ/mol	Joback Method
hf	-1288.45	kJ/mol	Joback Method
hfus	22.78	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.823		Crippen Method
mcvol	136.080	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	557.52	K	Joback Method
tc	750.93	K	Joback Method
tf	384.22	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.58	J/mol×K	557.52	Joback Method
cpg	353.68	J/mol×K	589.75	Joback Method
cpg	362.97	J/mol×K	621.99	Joback Method
cpg	371.51	J/mol×K	654.22	Joback Method
cpg	379.36	J/mol×K	686.46	Joback Method
cpg	386.55	J/mol×K	718.69	Joback Method
cpg	393.14	J/mol×K	750.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22227265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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