3-(Trifluoromethoxy)benzamide

Inchi: InChI=1S/C8H6F3NO2/c9-8(10,11)14-6-3-1-2-5(4-6)7(12)13/h1-4H,(H2,12,13)
InchiKey: RRANUIMYSXUNCN-UHFFFAOYSA-N
Formula: C8H6F3NO2
SMILES: NC(=O)c1cccc(OC(F)(F)F)c1
Mol. weight [g/mol]: 205.13
CAS: 658-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-629.80	kJ/mol	Joback Method
hf	-791.48	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.684		Crippen Method
mcvol	122.550	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	557.50	K	Joback Method
tc	768.33	K	Joback Method
tf	378.47	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.64	J/mol×K	557.50	Joback Method
cpg	303.82	J/mol×K	592.64	Joback Method
cpg	313.28	J/mol×K	627.78	Joback Method
cpg	322.04	J/mol×K	662.91	Joback Method
cpg	330.13	J/mol×K	698.05	Joback Method
cpg	337.58	J/mol×K	733.19	Joback Method
cpg	344.43	J/mol×K	768.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C658913&Units=SI

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