2,3,4-Trifluorobenzamide

Inchi: InChI=1S/C7H4F3NO/c8-4-2-1-3(7(11)12)5(9)6(4)10/h1-2H,(H2,11,12)
InchiKey: XGOGYOBKQVLGAY-UHFFFAOYSA-N
Formula: C7H4F3NO
SMILES: NC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 175.11
CAS: 207919-09-3

Physical Properties

Property code	Value	Unit	Source
gf	-555.32	kJ/mol	Joback Method
hf	-652.81	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	50.37	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.203		Crippen Method
mcvol	102.590	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	525.39	K	Joback Method
tc	731.08	K	Joback Method
tf	367.59	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.20	J/mol×K	525.39	Joback Method
cpg	232.23	J/mol×K	559.67	Joback Method
cpg	239.81	J/mol×K	593.95	Joback Method
cpg	246.96	J/mol×K	628.23	Joback Method
cpg	253.67	J/mol×K	662.52	Joback Method
cpg	259.97	J/mol×K	696.80	Joback Method
cpg	265.86	J/mol×K	731.08	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=C207919093&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume