m-Trifluoromethoxybenzoic acid

Other names: Benzoic acid, 3-(trifluoromethoxy)-
3-(trifluoromethoxy)benzoic acid
Inchi: InChI=1S/C8H5F3O3/c9-8(10,11)14-6-3-1-2-5(4-6)7(12)13/h1-4H,(H,12,13)
InchiKey: OKPFIWIMBJNFSE-UHFFFAOYSA-N
Formula: C8H5F3O3
SMILES: O=C(O)c1cccc(OC(F)(F)F)c1
Mol. weight [g/mol]: 206.12
CAS: 1014-81-9

Physical Properties

Property code	Value	Unit	Source
gf	-833.07	kJ/mol	Joback Method
hf	-977.50	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.283		Crippen Method
mcvol	118.440	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	577.15	K	Joback Method
tc	766.26	K	Joback Method
tf	356.03	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.22	J/mol×K	577.15	Joback Method
cpg	294.59	J/mol×K	608.67	Joback Method
cpg	302.41	J/mol×K	640.19	Joback Method
cpg	309.69	J/mol×K	671.71	Joback Method
cpg	316.46	J/mol×K	703.23	Joback Method
cpg	322.74	J/mol×K	734.74	Joback Method
cpg	328.56	J/mol×K	766.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1014819&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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