3-(Trifluoromethoxy)benzoic acid

Other names: 3-(trifluoromethoxy)benzoic acid
Benzoic acid, 3-(trifluoromethoxy)-
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

Physical Properties

Property code	Value	Unit	Source
af	0.7082		Cheméo Relay (1.0)
gf	-833.07	kJ/mol	Joback Method
hf	-1117.71	kJ/mol	Cheméo Relay (1.0)
hfus	18.83	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Cheméo Relay (1.0)
ie	9.95	eV	Cheméo Relay (1.0)
log10ws	-2.71		Cheméo Relay (1.0)
logp	2.283		Crippen Method
mcvol	118.440	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	499.09	K	Cheméo Relay (1.0)
tc	681.67	K	Cheméo Relay (1.0)
tf	325.48	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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