3-(Trifluoromethyl)benzoic acid

Other names:	«alpha»,«alpha»,«alpha»-Trifluoro-m-toluic acid
	m-Trifluoromethylbenzoic acid
	Benzoic acid, 3-(trifluoromethyl)-
	m-Toluic acid, «alpha»,«alpha»,«alpha»-trifluoro-
	Benzoic acid, trifluoromethyl-
	m-Trifluorometylbenzoic acid
Inchi:	InChI=1S/C8H5F3O2/c9-8(10,11)6-3-1-2-5(4-6)7(12)13/h1-4H,(H,12,13)
InchiKey:	FQXQBFUUVCDIRK-UHFFFAOYSA-N
Formula:	C8H5F3O2
SMILES:	O=C(O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	190.12
CAS:	454-92-2

Physical Properties

Property code	Value	Unit	Source
chs	-3329.80 ± 0.59	kJ/mol	NIST Webbook
chs	-3377.00	kJ/mol	NIST Webbook
gf	-728.07	kJ/mol	Joback Method
hf	-845.28	kJ/mol	Joback Method
hfs	-1069.70 ± 1.20	kJ/mol	NIST Webbook
hfus	17.64	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.404		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	554.73	K	Joback Method
tc	745.16	K	Joback Method
tf	375.00 ± 5.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	301.53	J/mol×K	713.42	Joback Method
cpg	264.67	J/mol×K	554.73	Joback Method
cpg	273.20	J/mol×K	586.47	Joback Method
cpg	281.11	J/mol×K	618.21	Joback Method
cpg	288.45	J/mol×K	649.94	Joback Method
cpg	295.25	J/mol×K	681.68	Joback Method
cpg	307.35	J/mol×K	745.16	Joback Method
cps	223.60	J/mol×K	298.15	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	511.70	K	103.00	NIST Webbook
tbrp	511.60	K	103.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C454922&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume