2-Trifluoromethylbenzoic acid

Other names: 2-(Trifluoromethyl)benzoic acid
Benzoic acid, 2-(trifluoromethyl)-
o-Trifluoromethylbenzoic acid
Inchi: InChI=1S/C8H5F3O2/c9-8(10,11)6-4-2-1-3-5(6)7(12)13/h1-4H,(H,12,13)
InchiKey: FBRJYBGLCHWYOE-UHFFFAOYSA-N
Formula: C8H5F3O2
SMILES: O=C(O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 190.12

Physical Properties

Property code	Value	Unit	Source
hf	-942.49	kJ/mol	Cheméo Relay (1.0)
hfus	17.64	kJ/mol	Joback Method
hvap	74.47	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
log10ws	-1.60		Aqueous Solubility Prediction Method
logp	2.404		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
tb	495.75	K	Cheméo Relay (1.0)
tc	702.78	K	Cheméo Relay (1.0)
tf	344.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	301.53	J/mol×K	713.42	Joback Method
cpg	307.35	J/mol×K	745.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	520.20	K	100.00	NIST Webbook
tbrp	520.00	K	100.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C433976&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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.