

«alpha», «alpha», «alpha»-Trifluoro-o-toluic acid

Other names:	2-(Trifluoromethyl)benzoic acid 2-Trifluoromethylbenzoic 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
CAS:	433-97-6

Physical Properties

Property code	Value	Unit	Source
gf	-728.07	kJ/mol	Joback Method
hf	-845.28	kJ/mol	Joback Method
hfus	17.64	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-1.60		Aqueous Solubility Prediction 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	333.80	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.67	J/molxK	554.73	Joback Method
cpg	273.20	J/molxK	586.47	Joback Method
cpg	281.11	J/molxK	618.21	Joback Method
cpg	288.45	J/molxK	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

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/15-510-8/alpha-alpha-alpha-Trifluoro-o-toluic-acid.pdf>

Generated by Cheméo on 2024-04-27 10:12:39.879052813 +0000 UTC m=+16502008.799630134.

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