M-(FLUOROSULFONYL)BENZOIC ACID

Other names: Benzoic acid, 3-(fluorosulfonyl)-
m-(Fluorosulfonyl)benzoic acid
3-(fluorosulphonyl)benzoic acid
Inchi: InChI=1S/C7H5FO4S/c8-13(11,12)6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
InchiKey: VWYMBWGOJRULOV-UHFFFAOYSA-N
Formula: C7H5FO4S
SMILES: O=C(O)c1cccc(S(=O)(=O)F)c1
Mol. weight [g/mol]: 204.18

Physical Properties

Property code	Value	Unit	Source
af	0.7310		Cheméo Relay (1.0)
gf	-818.25	kJ/mol	Joback Method
hf	-817.06	kJ/mol	Cheméo Relay (1.0)
hfus	27.68	kJ/mol	Joback Method
hvap	101.96	kJ/mol	Cheméo Relay (1.0)
ie	10.43	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	1.043		Crippen Method
mcvol	123.030	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
tb	561.21	K	Cheméo Relay (1.0)
tc	824.09	K	Cheméo Relay (1.0)
tf	457.93	K	Cheméo Relay (1.0)
vc	0.426	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.17	J/mol×K	584.32	Joback Method
cpg	283.53	J/mol×K	616.69	Joback Method
cpg	291.35	J/mol×K	649.05	Joback Method
cpg	298.65	J/mol×K	681.42	Joback Method
cpg	305.42	J/mol×K	713.79	Joback Method

cpg	311.67	J/mol×K	746.15	Joback Method
cpg	317.39	J/mol×K	778.52	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C454955&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

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