

O-fluorophenylacetic acid

Other names:	o-Fluorophenylacetic acid 2-Fluorophenylacetic acid Acetic acid, (o-fluorophenyl)-
Inchi:	InChI=1S/C8H7FO2/c9-7-4-2-1-3-6(7)5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	RPTRFSADOICSSK-UHFFFAOYSA-N
Formula:	C8H7FO2
SMILES:	O=C(O)Cc1ccccc1F
Mol. weight [g/mol]:	154.14

Physical Properties

Property code	Value	Unit	Source
hfus	18.89	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Cheméo Relay (1.0)
ie	8.84	eV	Cheméo Relay (1.0)
log10ws	-1.27		Cheméo Relay (1.0)
logp	1.453		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	523.75	K	Cheméo Relay (1.0)
tf	370.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.17	J/mol×K	559.42	Joback Method
cpg	253.02	J/mol×K	592.36	Joback Method
cpg	261.35	J/mol×K	625.29	Joback Method
cpg	269.17	J/mol×K	658.23	Joback Method
cpg	276.51	J/mol×K	691.16	Joback Method
cpg	283.38	J/mol×K	724.10	Joback Method
cpg	289.80	J/mol×K	757.03	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C451821&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

cpg:	Ideal gas heat capacity
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
tf:	Normal melting (fusion) point

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