

2-CHLORO-6-FLUOROPHENYLACETIC ACID

Other names:	Benzeneacetic acid, 2-chloro-6-fluoro-
Inchi:	InChI=1S/C8H6ClFO2/c9-6-2-1-3-7(10)5(6)4-8(11)12/h1-3H,4H2,(H,11,12)
InchiKey:	GUAIAAXDEJZRBP-UHFFFAOYSA-N
Formula:	C8H6ClFO2
SMILES:	O=C(O)Cc1c(F)cccc1Cl
Mol. weight [g/mol]:	188.59

Physical Properties

Property code	Value	Unit	Source
hfus	22.70	kJ/mol	Joback Method
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-2.09		Cheméo Relay (1.0)
logp	2.106		Crippen Method
mcvol	121.270	ml/mol	McGowan Method
tb	542.43	K	Cheméo Relay (1.0)
tf	399.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.37	J/mol×K	601.83	Joback Method
cpg	272.31	J/mol×K	635.63	Joback Method
cpg	279.76	J/mol×K	669.43	Joback Method
cpg	286.74	J/mol×K	703.23	Joback Method
cpg	293.27	J/mol×K	737.03	Joback Method
cpg	299.36	J/mol×K	770.84	Joback Method
cpg	305.03	J/mol×K	804.64	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C37777767&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/ci990307I>

Legend

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

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