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]: 188.58
CAS: 37777-76-7

Physical Properties

Property code	Value	Unit	Source
gf	-362.85	kJ/mol	Joback Method
hf	-471.52	kJ/mol	Joback Method
hfus	22.70	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.106		Crippen Method
mcvol	121.270	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	601.83	K	Joback Method
tc	804.64	K	Joback Method
tf	372.64	K	Joback Method
vc	0.468	m3/kmol	Joback Method

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37777767&Units=SI
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/22-933-1/2-Chloro-6-fluorophenylacetic-acid.pdf
Generated by Cheméo on 2024-04-27 02:12:48.129235188 +0000 UTC m=+16473217.049812504.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.