2-CHLORO-6-FLUOROBENZOIC ACID

Other names: Benzoic acid, 2-chloro-6-fluoro-
Inchi: InChI=1S/C7H4ClFO2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H,10,11)
InchiKey: XNTIGDVFBDJLTQ-UHFFFAOYSA-N
Formula: C7H4ClFO2
SMILES: O=C(O)c1c(F)cccc1Cl
Mol. weight [g/mol]: 174.56

Physical Properties

Property code	Value	Unit	Source
hf	-497.42	kJ/mol	Cheméo Relay (1.0)
hfus	20.11	kJ/mol	Joback Method
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	2.177		Crippen Method
mcvol	107.180	ml/mol	McGowan Method
tb	521.57	K	Cheméo Relay (1.0)
tf	385.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.54	J/mol×K	578.95	Joback Method
cpg	227.48	J/mol×K	613.26	Joback Method
cpg	233.97	J/mol×K	647.58	Joback Method
cpg	240.04	J/mol×K	681.89	Joback Method
cpg	245.70	J/mol×K	716.20	Joback Method
cpg	250.97	J/mol×K	750.52	Joback Method
cpg	255.86	J/mol×K	784.83	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C434753&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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
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