2,4-DIFLUOROPHENYLACETIC ACID

Other names: Benzeneacetic acid, 2,4-difluoro-
Inchi: InChI=1S/C8H6F2O2/c9-6-2-1-5(3-8(11)12)7(10)4-6/h1-2,4H,3H2,(H,11,12)
InchiKey: QPKZIGHNRLZBCL-UHFFFAOYSA-N
Formula: C8H6F2O2
SMILES: O=C(O)Cc1ccc(F)cc1F
Mol. weight [g/mol]: 172.13

Physical Properties

Property code	Value	Unit	Source
hfus	21.59	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-1.71		Cheméo Relay (1.0)
logp	1.592		Crippen Method
mcvol	110.800	ml/mol	McGowan Method
tb	516.12	K	Cheméo Relay (1.0)
tf	380.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.48	J/mol×K	563.67	Joback Method
cpg	259.65	J/mol×K	595.28	Joback Method
cpg	267.37	J/mol×K	626.88	Joback Method
cpg	274.66	J/mol×K	658.49	Joback Method
cpg	281.52	J/mol×K	690.09	Joback Method
cpg	287.98	J/mol×K	721.70	Joback Method
cpg	294.04	J/mol×K	753.30	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81228093&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point