2,6-Difluorophenylacetic acid

Other names: Benzeneacetic acid, 2,6-difluoro-
Inchi: InChI=1S/C8H6F2O2/c9-6-2-1-3-7(10)5(6)4-8(11)12/h1-3H,4H2,(H,11,12)
InchiKey: FUGDCKXBUZFEON-UHFFFAOYSA-N
Formula: C8H6F2O2
SMILES: O=C(O)Cc1c(F)cccc1F
Mol. weight [g/mol]: 172.13
CAS: 85068-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-545.73	kJ/mol	Joback Method
hf	-651.89	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.592		Crippen Method
mcvol	110.800	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	563.67	K	Joback Method
tc	753.30	K	Joback Method
tf	343.31	K	Joback Method
vc	0.436	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C85068286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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