3,4-Difluorobenzoic acid

Other names: Benzoic acid, 3,4-difluoro-
Inchi: InChI=1S/C7H4F2O2/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3H,(H,10,11)
InchiKey: FPENCTDAQQQKNY-UHFFFAOYSA-N
Formula: C7H4F2O2
SMILES: O=C(O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 158.10
CAS: 455-86-7

Physical Properties

Property code	Value	Unit	Source
gf	-554.15	kJ/mol	Joback Method
hf	-631.25	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.663		Crippen Method
mcvol	96.710	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	540.79	K	Joback Method
tc	732.76	K	Joback Method
tf	332.04	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.83	J/mol×K	540.79	Joback Method
cpg	215.99	J/mol×K	572.79	Joback Method
cpg	222.74	J/mol×K	604.78	Joback Method
cpg	229.10	J/mol×K	636.78	Joback Method
cpg	235.09	J/mol×K	668.77	Joback Method
cpg	240.70	J/mol×K	700.77	Joback Method
cpg	245.97	J/mol×K	732.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C455867&Units=SI

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