2,5-Difluorobenzoic acid, ethyl ester

Inchi: InChI=1S/C9H8F2O2/c1-2-13-9(12)7-5-6(10)3-4-8(7)11/h3-5H,2H2,1H3
InchiKey: VTNZLYJCCASTNV-UHFFFAOYSA-N
Formula: C9H8F2O2
SMILES: CCOC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 186.16

Physical Properties

Property code	Value	Unit	Source
gf	-505.49	kJ/mol	Joback Method
hf	-652.52	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	46.75	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.142		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
tb	516.79	K	Joback Method
tc	714.01	K	Joback Method
tf	315.99	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.63	J/mol×K	516.79	Joback Method
cpg	283.34	J/mol×K	549.66	Joback Method
cpg	293.54	J/mol×K	582.53	Joback Method
cpg	303.24	J/mol×K	615.40	Joback Method
cpg	312.44	J/mol×K	648.27	Joback Method
cpg	321.15	J/mol×K	681.14	Joback Method
cpg	329.36	J/mol×K	714.01	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=U338799&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume