3,4-Difluorobenzoic acid, propyl ester

Inchi: InChI=1S/C10H10F2O2/c1-2-5-14-10(13)7-3-4-8(11)9(12)6-7/h3-4,6H,2,5H2,1H3
InchiKey: MIRZUZXOHWPGEL-UHFFFAOYSA-N
Formula: C10H10F2O2
SMILES: CCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 200.18

Physical Properties

Property code	Value	Unit	Source
gf	-497.07	kJ/mol	Joback Method
hf	-673.16	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.532		Crippen Method
mcvol	138.980	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
tb	539.67	K	Joback Method
tc	734.29	K	Joback Method
tf	327.26	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.53	J/mol×K	539.67	Joback Method
cpg	328.23	J/mol×K	572.11	Joback Method
cpg	339.37	J/mol×K	604.54	Joback Method
cpg	349.95	J/mol×K	636.98	Joback Method
cpg	359.98	J/mol×K	669.42	Joback Method
cpg	369.46	J/mol×K	701.85	Joback Method
cpg	378.41	J/mol×K	734.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338858&Units=SI
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

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