2,4-Difluorobenzoic acid, butyl ester

Inchi: InChI=1S/C11H12F2O2/c1-2-3-6-15-11(14)9-5-4-8(12)7-10(9)13/h4-5,7H,2-3,6H2,1H3
InchiKey: PVQBFMMTUNVXJG-UHFFFAOYSA-N
Formula: C11H12F2O2
SMILES: CCCCOC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 214.21

Physical Properties

Property code	Value	Unit	Source
gf	-488.65	kJ/mol	Joback Method
hf	-693.80	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.922		Crippen Method
mcvol	153.070	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	562.55	K	Joback Method
tc	754.68	K	Joback Method
tf	338.53	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.28	J/mol×K	562.55	Joback Method
cpg	374.85	J/mol×K	594.57	Joback Method
cpg	386.80	J/mol×K	626.59	Joback Method
cpg	398.16	J/mol×K	658.62	Joback Method
cpg	408.92	J/mol×K	690.64	Joback Method
cpg	419.09	J/mol×K	722.66	Joback Method
cpg	428.68	J/mol×K	754.68	Joback Method

Sources

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=U338781&Units=SI
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
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