2-Fluorobenzoic acid, butyl ester

Inchi: InChI=1S/C11H13FO2/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h4-7H,2-3,8H2,1H3
InchiKey: FJBYSTBVNZDKFV-UHFFFAOYSA-N
Formula: C11H13FO2
SMILES: CCCCOC(=O)c1ccccc1F
Mol. weight [g/mol]: 196.22

Physical Properties

Property code	Value	Unit	Source
gf	-284.21	kJ/mol	Joback Method
hf	-486.22	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.783		Crippen Method
mcvol	151.300	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	1428.00		NIST Webbook
tb	558.30	K	Joback Method
tc	758.64	K	Joback Method
tf	325.42	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.38	J/mol×K	558.30	Joback Method
cpg	367.84	J/mol×K	591.69	Joback Method
cpg	380.61	J/mol×K	625.08	Joback Method
cpg	392.68	J/mol×K	658.47	Joback Method
cpg	404.08	J/mol×K	691.86	Joback Method
cpg	414.82	J/mol×K	725.25	Joback Method
cpg	424.91	J/mol×K	758.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372953&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

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