Propyl 2-fluorobenzoate

Other names: Benzoic acid, 2-fluoro-, propyl ester
2-Fluorobenzoic acid, propyl ester
Inchi: InChI=1S/C10H11FO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6H,2,7H2,1H3
InchiKey: IOQAFIPZQVBMTK-UHFFFAOYSA-N
Formula: C10H11FO2
SMILES: CCCOC(=O)c1ccccc1F
Mol. weight [g/mol]: 182.19
CAS: 811465-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-292.63	kJ/mol	Joback Method
hf	-465.58	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.393		Crippen Method
mcvol	137.210	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1324.00		NIST Webbook
tb	535.42	K	Joback Method
tc	738.70	K	Joback Method
tf	314.15	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.55	J/mol×K	535.42	Joback Method
cpg	321.15	J/mol×K	569.30	Joback Method
cpg	333.10	J/mol×K	603.18	Joback Method
cpg	344.41	J/mol×K	637.06	Joback Method
cpg	355.08	J/mol×K	670.94	Joback Method
cpg	365.13	J/mol×K	704.82	Joback Method

cpg	374.58	J/mol×K	738.70	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=C811465802&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume