3,4-Difluorobenzoic acid, pentyl ester

Inchi: InChI=1S/C12H14F2O2/c1-2-3-4-7-16-12(15)9-5-6-10(13)11(14)8-9/h5-6,8H,2-4,7H2,1H
InchiKey: YZDIGULCYRSDTH-UHFFFAOYSA-N
Formula: C12H14F2O2
SMILES: CCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-480.23	kJ/mol	Joback Method
hf	-714.44	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.312		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	585.43	K	Joback Method
tc	775.25	K	Joback Method
tf	349.80	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.77	J/mol×K	585.43	Joback Method
cpg	423.10	J/mol×K	617.07	Joback Method
cpg	435.78	J/mol×K	648.70	Joback Method
cpg	447.81	J/mol×K	680.34	Joback Method
cpg	459.21	J/mol×K	711.97	Joback Method
cpg	469.98	J/mol×K	743.61	Joback Method
cpg	480.13	J/mol×K	775.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338861&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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