

Carbonic acid, butyl 3,5-difluophenyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C11H12F2O3/c1-2-3-4-15-11(14)16-10-6-8(12)5-9(13)7-10/h5-7H,2-4H2,1H3

ONTQCNINZVWURQ-UHFFFAOYSA-N

C11H12F2O3

CCCCOC(=O)Oc1cc(F)cc(F)c1

230.21

Physical Properties

Property code	Value	Unit	Source
gf	-593.65	kJ/mol	Joback Method
hf	-826.02	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.280		Crippen Method
mcvol	158.940	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1341.00		NIST Webbook
tb	584.97	K	Joback Method
tc	775.71	K	Joback Method
tf	360.76	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.68	J/molxK	584.97	Joback Method
cpg	399.08	J/molxK	616.76	Joback Method
cpg	410.91	J/molxK	648.55	Joback Method
cpg	422.15	J/molxK	680.34	Joback Method
cpg	432.80	J/molxK	712.13	Joback Method
cpg	442.88	J/molxK	743.92	Joback Method
cpg	452.36	J/molxK	775.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U357841&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

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