3-Fluorobenzoic acid, 3,5-difluorophenyl ester

Inchi: InChI=1S/C13H7F3O2/c14-9-3-1-2-8(4-9)13(17)18-12-6-10(15)5-11(16)7-12/h1-7H
InchiKey: INKWJDUDXIXGOJ-UHFFFAOYSA-N
Formula: C13H7F3O2
SMILES: O=C(Oc1cc(F)cc(F)c1)c1cccc(F)c1
Mol. weight [g/mol]: 252.19

Physical Properties

Property code	Value	Unit	Source
gf	-563.84	kJ/mol	Joback Method
hf	-706.13	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	57.78	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.323		Crippen Method
mcvol	159.260	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
tb	639.24	K	Joback Method
tc	856.53	K	Joback Method
tf	400.60	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.86	J/mol×K	639.24	Joback Method
cpg	399.84	J/mol×K	675.45	Joback Method
cpg	410.99	J/mol×K	711.67	Joback Method
cpg	421.33	J/mol×K	747.88	Joback Method
cpg	430.88	J/mol×K	784.10	Joback Method
cpg	439.66	J/mol×K	820.31	Joback Method
cpg	447.69	J/mol×K	856.53	Joback Method

Sources

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=U299054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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