3,4-Difluorobenzoic acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C13H6F4O2/c14-8-4-9(15)6-10(5-8)19-13(18)7-1-2-11(16)12(17)3-7/h1-6H
InchiKey: DDTYNYKFAFNJCY-UHFFFAOYSA-N
Formula: C13H6F4O2
SMILES: O=C(Oc1cc(F)cc(F)c1)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 270.18

Physical Properties

Property code	Value	Unit	Source
gf	-768.28	kJ/mol	Joback Method
hf	-913.71	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.462		Crippen Method
mcvol	161.030	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
tb	643.49	K	Joback Method
tc	852.13	K	Joback Method
tf	413.71	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.83	J/mol×K	643.49	Joback Method
cpg	406.05	J/mol×K	678.26	Joback Method
cpg	416.52	J/mol×K	713.04	Joback Method
cpg	426.28	J/mol×K	747.81	Joback Method
cpg	435.32	J/mol×K	782.58	Joback Method
cpg	443.67	J/mol×K	817.36	Joback Method
cpg	451.33	J/mol×K	852.13	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=U357706&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