2,6-Difluoro-3-methylbenzoic acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C14H8F4O2/c1-7-2-3-11(17)12(13(7)18)14(19)20-10-5-8(15)4-9(16)6-10/h2-6H

InchiKey: ZWBARDCJLIMXKP-UHFFFAOYSA-N

Formula: C14H8F4O2

SMILES: Cc1ccc(F)c(C(=O)Oc2cc(F)cc(F)c2)c1F

Mol. weight [g/mol]: 284.21

Physical Properties

Property code	Value	Unit	Source
gf	-769.49	kJ/mol	Joback Method
hf	-945.82	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.771		Crippen Method
mcvol	175.120	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	671.35	K	Joback Method
tc	877.84	K	Joback Method
tf	437.50	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.88	J/mol×K	671.35	Joback Method
cpg	454.58	J/mol×K	705.76	Joback Method
cpg	465.53	J/mol×K	740.18	Joback Method
cpg	475.75	J/mol×K	774.59	Joback Method
cpg	485.24	J/mol×K	809.01	Joback Method
cpg	494.01	J/mol×K	843.42	Joback Method
cpg	502.08	J/mol×K	877.84	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=U357676&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