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

Inchi: InChI=1S/C15H12F2O2/c1-9-5-10(2)7-12(6-9)19-15(18)11-3-4-13(16)14(17)8-11/h3-8H,1

InchiKey: GKASGLKRDPJYLF-UHFFFAOYSA-N

Formula: C15H12F2O2

SMILES: Cc1cc(C)cc(OC(=O)c2ccc(F)c(F)c2)c1

Mol. weight [g/mol]: 262.25

Physical Properties

Property code	Value	Unit	Source
gf	-361.82	kJ/mol	Joback Method
hf	-562.77	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.801		Crippen Method
mcvol	185.670	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1842.00		NIST Webbook
tb	690.71	K	Joback Method
tc	911.11	K	Joback Method
tf	435.07	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.74	J/mol×K	690.71	Joback Method
cpg	492.36	J/mol×K	727.44	Joback Method
cpg	505.05	J/mol×K	764.18	Joback Method
cpg	516.83	J/mol×K	800.91	Joback Method
cpg	527.72	J/mol×K	837.64	Joback Method
cpg	537.73	J/mol×K	874.38	Joback Method
cpg	546.89	J/mol×K	911.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357713&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

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