2,6-Difluoro-3-methylbenzoic acid, phenyl ester

Inchi: InChI=1S/C14H10F2O2/c1-9-7-8-11(15)12(13(9)16)14(17)18-10-5-3-2-4-6-10/h2-8H,1H3

InchiKey: LOLMGBOAXPTHMF-UHFFFAOYSA-N

Formula: C14H10F2O2

SMILES: Cc1ccc(F)c(C(=O)Oc2ccccc2)c1F

Mol. weight [g/mol]: 248.22

Physical Properties

Property code	Value	Unit	Source
gf	-360.61	kJ/mol	Joback Method
hf	-530.66	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	60.82	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.492		Crippen Method
mcvol	171.580	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1783.00		NIST Webbook
tb	662.85	K	Joback Method
tc	886.28	K	Joback Method
tf	411.28	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.07	J/mol×K	662.85	Joback Method
cpg	442.31	J/mol×K	700.09	Joback Method
cpg	454.63	J/mol×K	737.33	Joback Method
cpg	466.03	J/mol×K	774.57	Joback Method
cpg	476.55	J/mol×K	811.80	Joback Method
cpg	486.21	J/mol×K	849.04	Joback Method
cpg	495.04	J/mol×K	886.28	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=U357678&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