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

Inchi: InChI=1S/C16H14F2O2/c1-9-6-10(2)8-12(7-9)20-16(19)14-13(17)5-4-11(3)15(14)18/h4-8

InchiKey: LENIKJKGZAVHPV-UHFFFAOYSA-N

Formula: C16H14F2O2

SMILES: Cc1cc(C)cc(OC(=O)c2c(F)ccc(C)c2F)c1

Mol. weight [g/mol]: 276.28

Physical Properties

Property code	Value	Unit	Source
gf	-363.03	kJ/mol	Joback Method
hf	-594.88	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.109		Crippen Method
mcvol	199.760	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	718.57	K	Joback Method
tc	936.27	K	Joback Method
tf	458.86	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.77	J/mol×K	718.57	Joback Method
cpg	543.73	J/mol×K	754.85	Joback Method
cpg	556.75	J/mol×K	791.14	Joback Method
cpg	568.84	J/mol×K	827.42	Joback Method
cpg	580.03	J/mol×K	863.71	Joback Method
cpg	590.32	J/mol×K	899.99	Joback Method
cpg	599.74	J/mol×K	936.27	Joback Method

Sources

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=U357683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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