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

Inchi: InChI=1S/C20H14F2O2/c1-13-11-12-16(21)18(19(13)22)20(23)24-17-10-6-5-9-15(17)14-

InchiKey: KDIJSKFJHNUAOQ-UHFFFAOYSA-N

Formula: C20H14F2O2

SMILES: Cc1ccc(F)c(C(=O)Oc2ccccc2-c2ccccc2)c1F

Mol. weight [g/mol]: 324.32

Physical Properties

Property code	Value	Unit	Source
gf	-207.31	kJ/mol	Joback Method
hf	-429.44	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	77.11	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	5.159		Crippen Method
mcvol	232.360	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	2379.00		NIST Webbook
tb	831.79	K	Joback Method
tc	1071.39	K	Joback Method
tf	517.84	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.19	J/mol×K	831.79	Joback Method
cpg	669.76	J/mol×K	871.72	Joback Method
cpg	682.07	J/mol×K	911.66	Joback Method
cpg	693.16	J/mol×K	951.59	Joback Method
cpg	703.10	J/mol×K	991.52	Joback Method
cpg	711.95	J/mol×K	1031.46	Joback Method
cpg	719.76	J/mol×K	1071.39	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=U343761&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