2,6-Difluoro-3-methylbenzoic acid, 4-isopropylphenyl ester

Inchi: InChI=1S/C17H16F2O2/c1-10(2)12-5-7-13(8-6-12)21-17(20)15-14(18)9-4-11(3)16(15)19

InchiKey: VKUDZDBNLGZXDH-UHFFFAOYSA-N

Formula: C17H16F2O2

SMILES: Cc1ccc(F)c(C(=O)Oc2ccc(C(C)C)cc2)c1F

Mol. weight [g/mol]: 290.30

Physical Properties

Property code	Value	Unit	Source
gf	-347.42	kJ/mol	Joback Method
hf	-609.33	kJ/mol	Joback Method
hfus	31.74	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.616		Crippen Method
mcvol	213.850	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook
tb	736.03	K	Joback Method
tc	953.47	K	Joback Method
tf	442.61	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.73	J/mol×K	736.03	Joback Method
cpg	599.46	J/mol×K	772.27	Joback Method
cpg	613.16	J/mol×K	808.51	Joback Method
cpg	625.85	J/mol×K	844.75	Joback Method
cpg	637.55	J/mol×K	880.99	Joback Method
cpg	648.29	J/mol×K	917.23	Joback Method
cpg	658.10	J/mol×K	953.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343758&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