2,5-Di(trifluoromethyl)benzoic acid, 4-isopropylphenyl ester

Inchi: InChI=1S/C18H14F6O2/c1-10(2)11-3-6-13(7-4-11)26-16(25)14-9-12(17(19,20)21)5-8-15

InchiKey: VBTOTMSSWKIZKW-UHFFFAOYSA-N

Formula: C18H14F6O2

SMILES: CC(C)c1ccc(OC(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)cc1

Mol. weight [g/mol]: 376.29

Physical Properties

Property code	Value	Unit	Source
gf	-1102.93	kJ/mol	Joback Method
hf	-1420.44	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.067		Crippen Method
mcvol	235.020	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	1814.00		NIST Webbook
tb	744.55	K	Joback Method
tc	946.71	K	Joback Method
tf	448.56	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.61	J/mol×K	744.55	Joback Method
cpg	689.06	J/mol×K	778.24	Joback Method
cpg	701.48	J/mol×K	811.94	Joback Method
cpg	712.96	J/mol×K	845.63	Joback Method
cpg	723.54	J/mol×K	879.32	Joback Method
cpg	733.31	J/mol×K	913.02	Joback Method
cpg	742.33	J/mol×K	946.71	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357371&Units=SI

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