2,5-Di(trifluoromethyl)benzoic acid, 3,4-dimethylphenyl ester

Inchi: InChI=1S/C17H12F6O2/c1-9-3-5-12(7-10(9)2)25-15(24)13-8-11(16(18,19)20)4-6-14(13)1

InchiKey: KLIBLEPXWRPPHQ-UHFFFAOYSA-N

Formula: C17H12F6O2

SMILES: Cc1ccc(OC(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)cc1C

Mol. weight [g/mol]: 362.27

Physical Properties

Property code	Value	Unit	Source
gf	-1118.54	kJ/mol	Joback Method
hf	-1405.99	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.560		Crippen Method
mcvol	220.930	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	727.09	K	Joback Method
tc	928.87	K	Joback Method
tf	464.81	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.42	J/mol×K	727.09	Joback Method
cpg	633.22	J/mol×K	760.72	Joback Method
cpg	645.05	J/mol×K	794.35	Joback Method
cpg	655.99	J/mol×K	827.98	Joback Method
cpg	666.08	J/mol×K	861.61	Joback Method
cpg	675.40	J/mol×K	895.24	Joback Method
cpg	683.99	J/mol×K	928.87	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=U357369&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