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

Inchi: InChI=1S/C16H10F6O2/c1-9-3-2-4-11(7-9)24-14(23)12-8-10(15(17,18)19)5-6-13(12)16(2

InchiKey: KMOKEJLRHGESTA-UHFFFAOYSA-N

Formula: C16H10F6O2

SMILES: Cc1cccc(OC(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)c1

Mol. weight [g/mol]: 348.24

Physical Properties

Property code	Value	Unit	Source
gf	-1117.33	kJ/mol	Joback Method
hf	-1373.88	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	59.41	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.252		Crippen Method
mcvol	206.840	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1635.00		NIST Webbook
tb	699.23	K	Joback Method
tc	902.34	K	Joback Method
tf	441.02	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.10	J/mol×K	699.23	Joback Method
cpg	581.67	J/mol×K	733.08	Joback Method
cpg	593.27	J/mol×K	766.93	Joback Method
cpg	603.95	J/mol×K	800.79	Joback Method
cpg	613.77	J/mol×K	834.64	Joback Method
cpg	622.79	J/mol×K	868.49	Joback Method
cpg	631.09	J/mol×K	902.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357744&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