2,4,5-Trifluoro-3-methoxybenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C16H13F3O3/c1-8-4-9(2)6-10(5-8)22-16(20)11-7-12(17)14(19)15(21-3)13(11)1

InchiKey: CTRNJGBDFLTKJH-UHFFFAOYSA-N

Formula: C16H13F3O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2cc(C)cc(C)c2)c1F

Mol. weight [g/mol]: 310.27

Physical Properties

Property code	Value	Unit	Source
gf	-672.47	kJ/mol	Joback Method
hf	-934.68	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	3.949		Crippen Method
mcvol	207.400	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2118.00		NIST Webbook
tb	745.24	K	Joback Method
tc	953.69	K	Joback Method
tf	494.20	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.47	J/mol×K	745.24	Joback Method
cpg	575.41	J/mol×K	779.98	Joback Method
cpg	587.47	J/mol×K	814.72	Joback Method
cpg	598.65	J/mol×K	849.47	Joback Method
cpg	608.94	J/mol×K	884.21	Joback Method
cpg	618.33	J/mol×K	918.95	Joback Method
cpg	626.82	J/mol×K	953.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357616&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