3-Trifluoromethylbenzoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C15H11F3O3/c1-20-12-5-7-13(8-6-12)21-14(19)10-3-2-4-11(9-10)15(16,17)18

InchiKey: IFNISUAKWTXQAB-UHFFFAOYSA-N

Formula: C15H11F3O3

SMILES: COc1ccc(OC(=O)c2cccc(C(F)(F)F)c2)cc1

Mol. weight [g/mol]: 296.24

Physical Properties

Property code	Value	Unit	Source
gf	-639.53	kJ/mol	Joback Method
hf	-876.91	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	62.68	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.933		Crippen Method
mcvol	193.310	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	699.21	K	Joback Method
tc	917.54	K	Joback Method
tf	435.27	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.20	J/mol×K	699.21	Joback Method
cpg	530.56	J/mol×K	735.60	Joback Method
cpg	542.88	J/mol×K	771.99	Joback Method
cpg	554.19	J/mol×K	808.37	Joback Method
cpg	564.54	J/mol×K	844.76	Joback Method
cpg	573.96	J/mol×K	881.15	Joback Method
cpg	582.49	J/mol×K	917.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307679&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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