Trifluoroacetic acid, 4-methoxyphenyl ester

Other names:	4-Methoxyphenol trifluoroacetate
	Acetic acid, trifluoro-, p-methoxyphenyl ester
	Trifluoroacetic acid, 4-methoxyphenyl ester
Inchi:	InChI=1S/C9H7F3O3/c1-14-6-2-4-7(5-3-6)15-8(13)9(10,11)12/h2-5H,1H3
InchiKey:	USKCDUZMASNBCQ-UHFFFAOYSA-N
Formula:	C9H7F3O3
SMILES:	COc1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]:	220.15

Physical Properties

Property code	Value	Unit	Source
hf	-1022.40	kJ/mol	Cheméo Relay (1.0)
hfus	18.52	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	2.163		Crippen Method
mcvol	132.530	ml/mol	McGowan Method
tb	474.33	K	Cheméo Relay (1.0)
tf	297.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.45	J/mol×K	530.27	Joback Method
cpg	318.53	J/mol×K	563.03	Joback Method
cpg	328.98	J/mol×K	595.80	Joback Method
cpg	338.80	J/mol×K	628.56	Joback Method
cpg	348.01	J/mol×K	661.32	Joback Method
cpg	356.62	J/mol×K	694.09	Joback Method
cpg	364.65	J/mol×K	726.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5672877&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point