Methyl 3-trifluoroacetyloxybenzoate

Other names: m-Hydroxy benzoic acid, TFA-ME
Inchi: InChI=1S/C10H7F3O4/c1-16-8(14)6-3-2-4-7(5-6)17-9(15)10(11,12)13/h2-5H,1H3
InchiKey: DVZQVDADQBLOIT-UHFFFAOYSA-N
Formula: C10H7F3O4
SMILES: COC(=O)c1cccc(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 248.16

Physical Properties

Property code	Value	Unit	Source
gf	-913.33	kJ/mol	Joback Method
hf	-1111.35	kJ/mol	Joback Method
hfus	22.71	kJ/mol	Joback Method
hvap	55.36	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	1.941		Crippen Method
mcvol	148.190	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
tb	607.02	K	Joback Method
tc	808.77	K	Joback Method
tf	389.91	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.02	J/mol×K	607.02	Joback Method
cpg	377.74	J/mol×K	640.64	Joback Method
cpg	387.76	J/mol×K	674.27	Joback Method
cpg	397.08	J/mol×K	707.89	Joback Method
cpg	405.73	J/mol×K	741.52	Joback Method
cpg	413.72	J/mol×K	775.14	Joback Method

cpg	421.07	J/mol×K	808.77	Joback Method

Sources

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=U374621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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