Methyl 3-trifluoromethoxybenzoate

Inchi: InChI=1S/C9H7F3O3/c1-14-8(13)6-3-2-4-7(5-6)15-9(10,11)12/h2-5H,1H3
InchiKey: YWSQRIKZJLRGPT-UHFFFAOYSA-N
Formula: C9H7F3O3
SMILES: COC(=O)c1cccc(OC(F)(F)F)c1
Mol. weight [g/mol]: 220.15
CAS: 148438-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-792.83	kJ/mol	Joback Method
hf	-978.13	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	46.39	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.372		Crippen Method
mcvol	132.530	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	530.27	K	Joback Method
tc	726.85	K	Joback Method
tf	328.71	K	Joback Method
vc	0.516	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148438000&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume