Formic acid, (2,3,6-trifluorophenyl)methyl ester

Inchi: InChI=1S/C8H5F3O2/c9-6-1-2-7(10)8(11)5(6)3-13-4-12/h1-2,4H,3H2
InchiKey: RCDQDOHXUOHABJ-UHFFFAOYSA-N
Formula: C8H5F3O2
SMILES: O=COCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 190.12

Physical Properties

Property code	Value	Unit	Source
gf	-688.95	kJ/mol	Joback Method
hf	-812.46	kJ/mol	Joback Method
hfus	22.07	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.777		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1098.00		NIST Webbook
tb	492.95	K	Joback Method
tc	679.37	K	Joback Method
tf	309.90	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.54	J/mol×K	492.95	Joback Method
cpg	249.03	J/mol×K	524.02	Joback Method
cpg	257.18	J/mol×K	555.09	Joback Method
cpg	264.97	J/mol×K	586.16	Joback Method
cpg	272.41	J/mol×K	617.23	Joback Method
cpg	279.50	J/mol×K	648.30	Joback Method
cpg	286.24	J/mol×K	679.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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