Formic acid, (3-fluorophenyl)methyl ester

Inchi: InChI=1S/C8H7FO2/c9-8-3-1-2-7(4-8)5-11-6-10/h1-4,6H,5H2
InchiKey: ZTANPNVVMLPICD-UHFFFAOYSA-N
Formula: C8H7FO2
SMILES: O=COCc1cccc(F)c1
Mol. weight [g/mol]: 154.14

Physical Properties

Property code	Value	Unit	Source
gf	-280.07	kJ/mol	Joback Method
hf	-397.30	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.499		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
tb	484.45	K	Joback Method
tc	688.49	K	Joback Method
tf	283.68	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.21	J/mol×K	484.45	Joback Method
cpg	234.38	J/mol×K	518.46	Joback Method
cpg	244.03	J/mol×K	552.46	Joback Method
cpg	253.17	J/mol×K	586.47	Joback Method
cpg	261.81	J/mol×K	620.48	Joback Method
cpg	269.97	J/mol×K	654.48	Joback Method
cpg	277.64	J/mol×K	688.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368721&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

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