3-Ethylphenol, O-trifluoroacetyl-

Inchi: InChI=1S/C10H9F3O2/c1-2-7-4-3-5-8(6-7)15-9(14)10(11,12)13/h3-6H,2H2,1H3
InchiKey: SYFKLDCFOVATRI-UHFFFAOYSA-N
Formula: C10H9F3O2
SMILES: CCc1cccc(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 218.17

Physical Properties

Property code	Value	Unit	Source
gf	-679.41	kJ/mol	Joback Method
hf	-866.55	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	46.20	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.717		Crippen Method
mcvol	140.750	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1049.00		NIST Webbook
tb	530.73	K	Joback Method
tc	726.25	K	Joback Method
tf	317.75	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.54	J/mol×K	530.73	Joback Method
cpg	340.77	J/mol×K	563.32	Joback Method
cpg	352.26	J/mol×K	595.90	Joback Method
cpg	363.03	J/mol×K	628.49	Joback Method
cpg	373.10	J/mol×K	661.08	Joback Method
cpg	382.52	J/mol×K	693.66	Joback Method
cpg	391.31	J/mol×K	726.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374273&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume