2-Chloro-4-methoxyphenol, trifluoroacetate

Inchi: InChI=1S/C9H6ClF3O3/c1-15-5-2-3-7(6(10)4-5)16-8(14)9(11,12)13/h2-4H,1H3
InchiKey: NBNMHUODJBUULW-UHFFFAOYSA-N
Formula: C9H6ClF3O3
SMILES: COc1ccc(OC(=O)C(F)(F)F)c(Cl)c1
Mol. weight [g/mol]: 254.59

Physical Properties

Property code	Value	Unit	Source
gf	-814.39	kJ/mol	Joback Method
hf	-1005.34	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.816		Crippen Method
mcvol	144.770	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
tb	572.68	K	Joback Method
tc	774.86	K	Joback Method
tf	371.15	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.00	J/mol×K	572.68	Joback Method
cpg	341.06	J/mol×K	606.38	Joback Method
cpg	350.50	J/mol×K	640.07	Joback Method
cpg	359.35	J/mol×K	673.77	Joback Method
cpg	367.59	J/mol×K	707.47	Joback Method
cpg	375.26	J/mol×K	741.16	Joback Method
cpg	382.36	J/mol×K	774.86	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=U375949&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