m-Cresol, 6-chloro-«alpha»,«alpha»,«alpha»-trifluoro-

Inchi: InChI=1S/C7H4ClF3O/c8-5-2-1-4(3-6(5)12)7(9,10)11/h1-3,12H
InchiKey: SUIZARUATMVYRT-UHFFFAOYSA-N
Formula: C7H4ClF3O
SMILES: Oc1cc(C(F)(F)F)ccc1Cl
Mol. weight [g/mol]: 196.55
CAS: 40889-91-6

Physical Properties

Property code	Value	Unit	Source
gf	-637.30	kJ/mol	Joback Method
hf	-752.88	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	47.77	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.064		Crippen Method
mcvol	109.150	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	503.85	K	Joback Method
tc	718.90	K	Joback Method
tf	353.42	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.40	J/mol×K	503.85	Joback Method
cpg	244.23	J/mol×K	539.69	Joback Method
cpg	252.22	J/mol×K	575.53	Joback Method
cpg	259.45	J/mol×K	611.37	Joback Method
cpg	266.01	J/mol×K	647.21	Joback Method
cpg	271.98	J/mol×K	683.06	Joback Method
cpg	277.44	J/mol×K	718.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40889916&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume