Phenol, 4-(trifluoromethoxy)-

Other names: 4-Trifluoromethoxyphenol
p-(trifluoromethoxy)phenol
Inchi: InChI=1S/C7H5F3O2/c8-7(9,10)12-6-3-1-5(11)2-4-6/h1-4,11H
InchiKey: WDRJNKMAZMEYOF-UHFFFAOYSA-N
Formula: C7H5F3O2
SMILES: Oc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 178.11
CAS: 828-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-720.74	kJ/mol	Joback Method
hf	-857.89	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	45.13	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.291		Crippen Method
mcvol	102.780	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	483.86	K	Joback Method
tc	690.24	K	Joback Method
tf	333.21	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.97	J/mol×K	483.86	Joback Method
cpg	243.80	J/mol×K	518.26	Joback Method
cpg	252.81	J/mol×K	552.65	Joback Method
cpg	261.08	J/mol×K	587.05	Joback Method
cpg	268.66	J/mol×K	621.45	Joback Method
cpg	275.63	J/mol×K	655.84	Joback Method
cpg	282.05	J/mol×K	690.24	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=C828273&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume