Phenol, 2-(trifluoromethyl)-

Other names:	o-Cresol, «alpha»,«alpha»,«alpha»-trifluoro- o-(Trifluoromethoxy)phenol o-Hydroxybenzotrifluoride 2-(Trifluoromethyl)phenol «alpha»,«alpha»,«alpha»-Trifluoro-o-cresol 2-Hydroxybenzotrifluoride o-(Trifluoromethyl)phenol
Inchi:	InChI=1S/C7H5F3O/c8-7(9,10)5-3-1-2-4-6(5)11/h1-4,11H
InchiKey:	ZOQOPXVJANRGJZ-UHFFFAOYSA-N
Formula:	C7H5F3O
SMILES:	Oc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	162.11
CAS:	444-30-4

Physical Properties

Property code	Value	Unit	Source
gf	-615.74	kJ/mol	Joback Method
hf	-725.67	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	42.72	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.411		Crippen Method
mcvol	96.910	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	420.70	K	NIST Webbook
tb	420.50 ± 0.50	K	NIST Webbook
tc	669.45	K	Joback Method
tf	310.98	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.51	J/mol×K	461.44	Joback Method

cpg	222.79	J/mol×K	496.11	Joback Method
cpg	232.14	J/mol×K	530.78	Joback Method
cpg	240.62	J/mol×K	565.44	Joback Method
cpg	248.33	J/mol×K	600.11	Joback Method
cpg	255.34	J/mol×K	634.78	Joback Method
cpg	261.74	J/mol×K	669.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C444304&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