3,5-Bis(trifluoromethyl)phenol

Other names:	3,5-di(Trifluoromethyl)phenol
	Phenol, 3,5-bis(trifluoromethyl)-
	3,5-Xylenol, aplha,aplha,aplha,aplha',aplha',aplha'-hexafluoro-
	«alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-hexafluoro-3,5-xylenol
Inchi:	InChI=1S/C8H4F6O/c9-7(10,11)4-1-5(8(12,13)14)3-6(15)2-4/h1-3,15H
InchiKey:	ODSXJQYJADZFJX-UHFFFAOYSA-N
Formula:	C8H4F6O
SMILES:	Oc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	230.11
CAS:	349-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-1198.54	kJ/mol	Joback Method
hf	-1354.86	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	41.86	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.430		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	483.88	K	Joback Method
tc	671.98	K	Joback Method
tf	338.96	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.43	J/mol×K	483.88	Joback Method
cpg	291.63	J/mol×K	515.23	Joback Method
cpg	300.92	J/mol×K	546.58	Joback Method
cpg	309.37	J/mol×K	577.93	Joback Method
cpg	317.06	J/mol×K	609.28	Joback Method

cpg	324.05	J/mol×K	640.63	Joback Method
cpg	330.43	J/mol×K	671.98	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=C349586&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