2,3,4-Trifluorophenol

Other names: 2,3,4-Trifluorophenol
Inchi: InChI=1S/C6H3F3O/c7-3-1-2-4(10)6(9)5(3)8/h1-2,10H
InchiKey: IJGSULQFKYOYEU-UHFFFAOYSA-N
Formula: C6H3F3O
SMILES: Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 148.08

Physical Properties

Property code	Value	Unit	Source
af	0.4871		Cheméo Relay (1.0)
hfus	19.58	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Cheméo Relay (1.0)
ie	9.19 ± 0.02	eV	NIST Webbook
logp	1.810		Crippen Method
mcvol	82.820	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
rinpol	930.30		NIST Webbook
tb	423.23	K	Cheméo Relay (1.0)
tc	639.37	K	Cheméo Relay (1.0)
tf	292.80	K	Cheméo Relay (1.0)
vc	0.300	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.14	J/mol×K	451.75	Joback Method
cpg	178.30	J/mol×K	485.08	Joback Method
cpg	184.94	J/mol×K	518.40	Joback Method
cpg	191.10	J/mol×K	551.73	Joback Method
cpg	196.82	J/mol×K	585.05	Joback Method
cpg	202.14	J/mol×K	618.38	Joback Method
cpg	207.11	J/mol×K	651.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2822415&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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