

2,4,5-Trifluorophenol

Other names:	2,4,5-Trifluorophenol
Inchi:	InChI=1S/C6H3F3O/c7-3-1-5(9)6(10)2-4(3)8/h1-2,10H
InchiKey:	ODGMYCITQAIRCI-UHFFFAOYSA-N
Formula:	C6H3F3O
SMILES:	Oc1cc(F)c(F)cc1F
Mol. weight [g/mol]:	148.08

Physical Properties

Property code	Value	Unit	Source
af	0.4909		Cheméo Relay (1.0)
hf	-648.52	kJ/mol	Cheméo Relay (1.0)
hfus	19.58	kJ/mol	Joback Method
hvap	57.17	kJ/mol	Cheméo Relay (1.0)
ie	9.10 ± 0.02	eV	NIST Webbook
log10ws	-1.50		Cheméo Relay (1.0)
logp	1.810		Crippen Method
mcvol	82.820	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	421.19	K	Cheméo Relay (1.0)
tc	646.59	K	Cheméo Relay (1.0)
tf	323.66	K	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:	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=C2268168&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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