

p-Fluorophenyl trifluoromethyl ether

Other names:	Benzene, 1-fluoro-4-(trifluoromethoxy)- p, «alpha», «alpha», «alpha»-tetrafluoroanisole
Inchi:	InChI=1S/C7H4F4O/c8-5-1-3-6(4-2-5)12-7(9,10)11/h1-4H
InchiKey:	JULMJGDXANEQDP-UHFFFAOYSA-N
Formula:	C7H4F4O
SMILES:	Fc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	180.10
CAS:	352-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-770.56	kJ/mol	Joback Method
hf	-888.16	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	31.96	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.724		Crippen Method
mvol	98.680	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	407.49	K	Joback Method
tc	588.81	K	Joback Method
tf	234.60	K	Joback Method
vc	0.399	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.46	J/mol×K	407.49	Joback Method
cpg	206.19	J/mol×K	437.71	Joback Method
cpg	215.38	J/mol×K	467.93	Joback Method
cpg	224.03	J/mol×K	498.15	Joback Method
cpg	232.18	J/mol×K	528.37	Joback Method
cpg	239.83	J/mol×K	558.59	Joback Method
cpg	247.00	J/mol×K	588.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C352670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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

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