Trifluoromethoxybenzene

Other names: Benzene, (trifluoromethoxy)-
Trifluoromethoxybenzene
Inchi: InChI=1S/C7H5F3O/c8-7(9,10)11-6-4-2-1-3-5-6/h1-5H
InchiKey: GQHWSLKNULCZGI-UHFFFAOYSA-N
Formula: C7H5F3O
SMILES: FC(F)(F)Oc1ccccc1
Mol. weight [g/mol]: 162.11

Physical Properties

Property code	Value	Unit	Source
af	0.3691		Cheméo Relay (1.0)
hf	-752.54	kJ/mol	Cheméo Relay (1.0)
hfus	10.94	kJ/mol	Joback Method
hvap	35.91	kJ/mol	Cheméo Relay (1.0)
ie	10.00	eV	NIST Webbook
log10ws	-2.38		Cheméo Relay (1.0)
logp	2.585		Crippen Method
mcvol	96.910	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	372.00 ± 1.00	K	NIST Webbook
tc	546.27	K	Cheméo Relay (1.0)
tf	172.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/mol×K	403.24	Joback Method
cpg	197.68	J/mol×K	434.92	Joback Method
cpg	207.79	J/mol×K	466.61	Joback Method
cpg	217.26	J/mol×K	498.29	Joback Method
cpg	226.13	J/mol×K	529.97	Joback Method
cpg	234.42	J/mol×K	561.66	Joback Method
cpg	242.15	J/mol×K	593.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C456553&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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