Trifluoromethanesulfonic anhydride

Other names:	Methanesulfonic acid, trifluoro-, anhydride trifluoromethanesulphonic anhydride
Inchi:	InChI=1S/C2F6O5S2/c3-1(4,5)14(9,10)13-15(11,12)2(6,7)8
InchiKey:	WJKHJLXJJJATHN-UHFFFAOYSA-N
Formula:	C2F6O5S2
SMILES:	O=S(=O)(OS(=O)(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	282.14
CAS:	358-23-6

Physical Properties

Property code	Value	Unit	Source
gf	-2239.30	kJ/mol	Joback Method
hf	-2317.69	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	0.702		Crippen Method
mcvol	111.710	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	356.50 ± 0.50	K	NIST Webbook
tc	486.63	K	Joback Method
tf	220.03	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.95	J/mol×K	352.30	Joback Method
cpg	236.03	J/mol×K	374.69	Joback Method
cpg	242.85	J/mol×K	397.08	Joback Method
cpg	249.39	J/mol×K	419.46	Joback Method
cpg	255.65	J/mol×K	441.85	Joback Method
cpg	261.64	J/mol×K	464.24	Joback Method
cpg	267.36	J/mol×K	486.63	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=C358236&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

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