

Trioxide, bis(trifluoromethyl)

Other names:	Bis(trifluoromethyl) trioxide Trifluoromethyl trioxide CF3O3CF3 bis(trifloromethyl) trioxide
Inchi:	InChI=1S/C2F6O3/c3-1(4,5)9-11-10-2(6,7)8
InchiKey:	JGFHBZWYOYWBRG-UHFFFAOYSA-N
Formula:	C2F6O3
SMILES:	FC(F)(F)OOOC(F)(F)F
Mol. weight [g/mol]:	186.01
CAS:	1718-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-1512.22	kJ/mol	Joback Method
hf	-1675.43	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	19.78	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.906		Crippen Method
mcvol	67.270	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	301.58	K	Joback Method
tc	435.29	K	Joback Method
tf	187.37	K	Joback Method
vc	0.287	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.77	J/mol×K	413.00	Joback Method
cpg	146.72	J/mol×K	301.58	Joback Method
cpg	151.47	J/mol×K	323.86	Joback Method
cpg	156.04	J/mol×K	346.15	Joback Method
cpg	160.45	J/mol×K	368.43	Joback Method

cpg	164.69	J/mol×K	390.72	Joback Method
cpg	172.69	J/mol×K	435.29	Joback Method
hvapt	24.30	kJ/mol	220.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1718189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
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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