

Ethane, 2-chloro-1,1,2-trifluoro-1-methoxy-

Other names:	Ether, 2-chloro-1,1,2-trifluoroethyl methyl 2-Chloro-1,1,2-trifluoroethyl methyl ether 1-Chloro-1,2,2-trifluoro-2-methoxyethane 2-chloro-1,1,2-trifluoro-1-methoxyethane
Inchi:	InChI=1S/C3H4ClF3O/c1-8-3(6,7)2(4)5/h2H,1H3
InchiKey:	KKXBMWAROXAWSZ-UHFFFAOYSA-N
Formula:	C3H4ClF3O
SMILES:	COC(F)(F)C(F)Cl
Mol. weight [g/mol]:	148.51
CAS:	425-87-6

Physical Properties

Property code	Value	Unit	Source
gf	-726.58	kJ/mol	Joback Method
hf	-855.57	kJ/mol	Joback Method
hfus	7.21	kJ/mol	Joback Method
hvap	34.53	kJ/mol	NIST Webbook
hvap	34.40 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.59		Crippen Method
logp	1.760		Crippen Method
mcpvol	76.550	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	343.40	K	NIST Webbook
tc	508.20	K	NIST Webbook
tf	164.91	K	Joback Method
vc	0.307	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.25	J/mol×K	322.03	Joback Method
cpg	139.60	J/mol×K	348.61	Joback Method
cpg	145.67	J/mol×K	375.19	Joback Method
cpg	151.45	J/mol×K	401.76	Joback Method

cpg	156.97	J/mol×K	428.34	Joback Method
cpg	162.22	J/mol×K	454.92	Joback Method
cpg	167.21	J/mol×K	481.50	Joback Method
hvapt	31.12	kJ/mol	343.40	NIST Webbook
hvapt	33.40 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	31.10 ± 0.10	kJ/mol	343.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.50	K	84.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C425876&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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