Ethane, 2-chloro-1-(chloromethoxy)-1,1,2-trifluoro-

Other names: Ether, chloromethyl 2-chloro-1,1,2-trifluoroethyl
Chloromethyl 2-chloro-1,1,2-trifluoroethyl ether
2-chloro-1-(chloromethoxy)-1,1,2-trifluoroethane
2-Chloro-1,1,2-trifluoroethyl chloromethyl ether

Inchi: InChI=1S/C3H3Cl2F3O/c4-1-9-3(7,8)2(5)6/h2H,1H2

InchiKey: FAERCLVMZOAFPK-UHFFFAOYSA-N

Formula: C3H3Cl2F3O

SMILES: FC(Cl)C(F)(F)OCCl

Mol. weight [g/mol]: 182.96

CAS: 428-92-2

Physical Properties

Property code	Value	Unit	Source
gf	-738.51	kJ/mol	Joback Method
hf	-871.31	kJ/mol	Joback Method
hfus	11.41	kJ/mol	Joback Method
hvap	42.40 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.24		Crippen Method
logp	2.327		Crippen Method
mcvol	88.790	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	359.46	K	Joback Method
tc	528.35	K	Joback Method
tf	194.83	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.22	J/mol×K	415.76	Joback Method
cpg	172.74	J/mol×K	443.90	Joback Method
cpg	177.96	J/mol×K	472.05	Joback Method
cpg	182.88	J/mol×K	500.20	Joback Method
cpg	155.22	J/mol×K	359.46	Joback Method

cpg	161.39	J/mol×K	387.61	Joback Method
cpg	187.52	J/mol×K	528.35	Joback Method
hvapt	41.20 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	40.10 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	39.00 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	37.80 ± 0.10	kJ/mol	358.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C428922&Units=SI

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