

2-Chloro-1,1,2-trifluoroethyl ethyl ether

Inchi:	InChI=1S/C4H6ClF3O/c1-2-9-4(7,8)3(5)6/h3H,2H2,1H3
InchiKey:	WOKICPFFJXCEDW-UHFFFAOYSA-N
Formula:	C4H6ClF3O
SMILES:	CCOC(F)(F)C(F)Cl
Mol. weight [g/mol]:	162.54
CAS:	310-71-4

Physical Properties

Property code	Value	Unit	Source
gf	-718.16	kJ/mol	Joback Method
hf	-876.21	kJ/mol	Joback Method
hfus	9.80	kJ/mol	Joback Method
hvap	37.63	kJ/mol	NIST Webbook
hvap	37.50 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.01		Crippen Method
logp	2.150		Crippen Method
mcvol	90.640	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	362.00	K	NIST Webbook
tc	524.40	K	NIST Webbook
tf	176.18	K	Joback Method
vc	0.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.61	J/mol×K	344.91	Joback Method
cpg	172.36	J/mol×K	371.59	Joback Method
cpg	179.76	J/mol×K	398.27	Joback Method
cpg	186.83	J/mol×K	424.95	Joback Method
cpg	193.58	J/mol×K	451.63	Joback Method
cpg	200.02	J/mol×K	478.31	Joback Method
cpg	206.15	J/mol×K	505.00	Joback Method
hvapt	32.57	kJ/mol	362.00	NIST Webbook

hvapt	36.50 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	35.30 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	34.20 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	32.90 ± 0.10	kJ/mol	358.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.00	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=C310714&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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