

Chloromethyl tert-butyl ether

Inchi: InChI=1S/C5H11ClO/c1-5(2,3)7-4-6/h4H2,1-3H3
InchiKey: CIACLSGBPZWWNK-UHFFFAOYSA-N
Formula: C5H11ClO
SMILES: CC(C)(C)OCCI
Mol. weight [g/mol]: 122.59

Physical Properties

Property code	Value	Unit	Source
gf	-122.87	kJ/mol	Joback Method
hf	-303.24	kJ/mol	Joback Method
hfus	6.68	kJ/mol	Joback Method
hvap	32.22	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.998		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	772.00		NIST Webbook
rinpol	772.00		NIST Webbook
tb	370.42	K	Joback Method
tc	555.51	K	Joback Method
tf	200.68	K	Joback Method
vc	0.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.93	J/molxK	370.42	Joback Method
cpg	184.03	J/molxK	401.27	Joback Method
cpg	193.67	J/molxK	432.12	Joback Method
cpg	202.87	J/molxK	462.97	Joback Method
cpg	211.63	J/molxK	493.82	Joback Method
cpg	219.98	J/molxK	524.67	Joback Method
cpg	227.93	J/molxK	555.51	Joback Method
dvisc	0.0061676	Paxs	200.68	Joback Method

dvisc	0.0027445	Paxs	228.97	Joback Method
dvisc	0.0014593	Paxs	257.26	Joback Method
dvisc	0.0008794	Paxs	285.55	Joback Method
dvisc	0.0005806	Paxs	313.84	Joback Method
dvisc	0.0004106	Paxs	342.13	Joback Method
dvisc	0.0003061	Paxs	370.42	Joback Method

Sources

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=R629142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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