1,2-DICHLOROETHYL ETHYL ETHER

Other names: Ether, 1,2-dichloroethyl ethyl
1,2-Dichloroethyl ethyl ether
1,2-Dichlorodiethyl ether
Ethyl 1,2-dichloroethyl ether
1,2-dichloro-2-ethoxyethane

Inchi: InChI=1S/C4H8Cl2O/c1-2-7-4(6)3-5/h4H,2-3H2,1H3

InchiKey: NNBUKAPOVBEMNI-UHFFFAOYSA-N

Formula: C4H8Cl2O

SMILES: CCOC(Cl)CCl

Mol. weight [g/mol]: 143.01

Physical Properties

Property code	Value	Unit	Source
hf	-328.07	kJ/mol	Cheméo Relay (1.0)
hfus	12.18	kJ/mol	Joback Method
hvap	42.98	kJ/mol	Cheméo Relay (1.0)
ie	10.44	eV	Cheméo Relay (1.0)
log10ws	-1.32		Cheméo Relay (1.0)
logp	1.827		Crippen Method
mcvol	97.570	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	865.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	856.00		NIST Webbook
tb	415.70	K	NIST Webbook
tb	418.20	K	NIST Webbook
tb	414.70 ± 0.60	K	NIST Webbook
tc	595.05	K	Cheméo Relay (1.0)
tf	219.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.62	J/mol×K	387.76	Joback Method

cpg	202.20	J/mol×K	574.35	Joback Method
cpg	196.06	J/mol×K	543.25	Joback Method
cpg	189.66	J/mol×K	512.15	Joback Method
cpg	183.02	J/mol×K	481.05	Joback Method
cpg	176.14	J/mol×K	449.96	Joback Method
cpg	169.00	J/mol×K	418.86	Joback Method
dvisc	0.0007863	Pa×s	294.84	Joback Method
dvisc	0.0002990	Pa×s	387.76	Joback Method
dvisc	0.0003902	Pa×s	356.78	Joback Method
dvisc	0.0005358	Pa×s	325.81	Joback Method
dvisc	0.0050358	Pa×s	201.91	Joback Method
dvisc	0.0012627	Pa×s	263.86	Joback Method
dvisc	0.0023000	Pa×s	232.89	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623461&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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