Bis(2-chloroethyl) ether

Other names:

1,1'-Oxybis(2-chloroethane)
1,5-Dichloro-3-oxapentane
1-Chloro-2-(«beta»-Chloroethoxy)ethane
1-Chloro-2-(Â«betaÂ»-Chloroethoxy)ethane
1-chloro-2-(2-chloroethoxy)ethane
2,2'-Dichloorethylether
2,2'-Dichlor-diaethylaether
2,2'-Dichlorethyl ether
2,2'-Dichlorodiethyl ether
2,2'-Dichlorodiethyl oxide
2,2'-Dichloroethyl ether
2,2'-Dicloroetiletere
2-Chloroethyl ether
BCEE
Beta,beta'-dichloroethyl ether
Bis(chloro-2-ethyl) oxide
Bis(«beta»-chloroethyl) ether
Bis(Â«betaÂ»-chloroethyl) ether
Chlorex
Chloroethyl ether
Clorex
DCEE
Di(2-chloroethyl) ether
Di(«beta»-chloroethyl) ether
Di(Â«betaÂ»-chloroethyl) ether
Dichloroether
Dichloroethyl ether
Dichloroethyl oxide
Diethylene glycol dichloride
Dwuchlorodwuetylowy eter
ENT 4,504
Ethane, 1,1'-oxybis[2-chloro-
Ether dichlore
Ether, bis(2-chloroethyl)
Ether, bis(chloroethyl)
Khloreks
NSC 406647
Oxyde de chlorethyle
Rcra waste number U025
UN 1916

s-Dichloroethyl ether
sym-Dichloroethyl ether
«beta»,«beta»'-Dichlorodiethyl ether
«beta»,«beta»'-Dichloroethyl ether
Â«betaÂ»,Â«betaÂ»'-Dichlorodiethyl ether
Â«betaÂ»,Â«betaÂ»'-Dichloroethyl ether

Inchi: InChI=1S/C4H8Cl2O/c5-1-3-7-4-2-6/h1-4H2
InchiKey: ZNSMNVMLTJELDZ-UHFFFAOYSA-N
Formula: C4H8Cl2O
SMILES: ClCCOCCCl
Mol. weight [g/mol]: 143.01
CAS: 111-44-4

Physical Properties

Property code	Value	Unit	Source
gf	-146.06	kJ/mol	Joback Method
hf	-289.59	kJ/mol	Joback Method
hfus	15.70	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-1.12		Aqueous Solubility Prediction Method
logp	1.481		Crippen Method
mcvol	97.570	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	984.00		NIST Webbook
rinpol	951.52		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	156.20		NIST Webbook
rinpol	945.90		NIST Webbook
rinpol	156.20		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1536.00		NIST Webbook

tb	452.25	K	NIST Webbook
tb	451.80 ± 0.40	K	NIST Webbook
tb	451.00 ± 2.00	K	NIST Webbook
tb	451.20	K	NIST Webbook
tb	451.00	K	NIST Webbook
tc	570.40	K	Joback Method
tf	227.05	K	NIST Webbook
tf	223.52	K	Aqueous Solubility Prediction Method
tf	226.25 ± 0.50	K	NIST Webbook
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.71	J/mol×K	509.67	Joback Method
cpg	175.62	J/mol×K	448.93	Joback Method
cpg	182.28	J/mol×K	479.30	Joback Method
cpg	200.87	J/mol×K	570.40	Joback Method
cpg	194.90	J/mol×K	540.04	Joback Method
cpg	161.62	J/mol×K	388.20	Joback Method
cpg	168.74	J/mol×K	418.57	Joback Method
cpl	253.00	J/mol×K	295.00	NIST Webbook
cpl	207.81	J/mol×K	293.15	NIST Webbook
dvisc	0.0017353	Pa×s	245.46	Joback Method
dvisc	0.0010643	Pa×s	274.01	Joback Method
dvisc	0.0007158	Pa×s	302.56	Joback Method
dvisc	0.0005155	Pa×s	331.10	Joback Method
dvisc	0.0003911	Pa×s	359.65	Joback Method
dvisc	0.0032180	Pa×s	216.91	Joback Method
dvisc	0.0003090	Pa×s	388.20	Joback Method
hfust	8.38	kJ/mol	226.50	NIST Webbook
hfust	8.39	kJ/mol	226.50	NIST Webbook
hfust	8.39	kJ/mol	226.50	NIST Webbook
hvapt	45.24	kJ/mol	273.00	NIST Webbook
hvapt	49.80	kJ/mol	374.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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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