

Benzene, (2-chloroethoxy)-

Other names:	Phenetole, «beta»-chloro- «beta»-Chlorophenetole (2-Chloroethoxy)benzene 1-Phenoxy-2-chloroethane 2-Chloroethyl phenyl ether 2-Phenoxyethyl chloride «beta»-Phenoxyethyl chloride
Inchi:	InChI=1S/C8H9ClO/c9-6-7-10-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	VQUYNUJARXBNPK-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	ClCCOc1ccccc1
Mol. weight [g/mol]:	156.61
CAS:	622-86-6

Physical Properties

Property code	Value	Unit	Source
gf	11.96	kJ/mol	Joback Method
hf	-119.88	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	42.47	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.304		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1190.20		NIST Webbook
tb	468.97	K	Joback Method
tc	683.94	K	Joback Method
tf	258.49	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	224.00	J/mol×K	468.97	Joback Method
cpg	276.92	J/mol×K	648.11	Joback Method
cpg	267.58	J/mol×K	612.28	Joback Method
cpg	257.64	J/mol×K	576.45	Joback Method
cpg	247.07	J/mol×K	540.63	Joback Method
cpg	235.86	J/mol×K	504.80	Joback Method
cpg	285.68	J/mol×K	683.94	Joback Method
dvisc	0.0002296	Pa×s	468.97	Joback Method
dvisc	0.0002918	Pa×s	433.89	Joback Method
dvisc	0.0003868	Pa×s	398.81	Joback Method
dvisc	0.0005415	Pa×s	363.73	Joback Method
dvisc	0.0008143	Pa×s	328.65	Joback Method
dvisc	0.0013502	Pa×s	293.57	Joback Method
dvisc	0.0025678	Pa×s	258.49	Joback Method

Sources

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=C622866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
vc: Critical Volume

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