

Benzene, 1-chloro-3-ethoxy-

Other names:	Phenetole, m-chloro- m-Chlorophenyl ethyl ether 1-chloro-3-ethoxybenzene
Inchi:	InChI=1S/C8H9ClO/c1-2-10-8-5-3-4-7(9)6-8/h3-6H,2H2,1H3
InchiKey:	HNMYS CABMYNGTP-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	CCOc1cccc(Cl)c1
Mol. weight [g/mol]:	156.61
CAS:	2655-83-6

Physical Properties

Property code	Value	Unit	Source
gf	2.33	kJ/mol	Joback Method
hf	-131.35	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	43.14	kJ/mol	Joback Method
ie	8.59 ± 0.15	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.739		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	473.95	K	Joback Method
tc	690.26	K	Joback Method
tf	271.01	K	Joback Method
vc	0.443	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.21	J/mol×K	473.95	Joback Method
cpg	235.63	J/mol×K	510.00	Joback Method
cpg	246.47	J/mol×K	546.05	Joback Method
cpg	256.73	J/mol×K	582.10	Joback Method
cpg	266.42	J/mol×K	618.15	Joback Method

cpg	275.56	J/molxK	654.20	Joback Method
cpg	284.16	J/molxK	690.26	Joback Method
dvisc	0.0018210	Paxs	271.01	Joback Method
dvisc	0.0010524	Paxs	304.83	Joback Method
dvisc	0.0006786	Paxs	338.66	Joback Method
dvisc	0.0004738	Paxs	372.48	Joback Method
dvisc	0.0003513	Paxs	406.30	Joback Method
dvisc	0.0002727	Paxs	440.13	Joback Method
dvisc	0.0002194	Paxs	473.95	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=C2655836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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