

Ethanesulfonyl chloride

Other names:	1-Ethanesulfonyl chloride Ethane sulfochloride Ethylsulfochloride Ethylsulfonyl chloride TL 77 ethanesulphonyl chloride
Inchi:	InChI=1S/C2H5ClO2S/c1-2-6(3,4)5/h2H2,1H3
InchiKey:	FRYHCSODNHYDPU-UHFFFAOYSA-N
Formula:	C2H5ClO2S
SMILES:	CCS(=O)(=O)Cl
Mol. weight [g/mol]:	128.58
CAS:	594-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-514.51	kJ/mol	Joback Method
hf	-553.70	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	43.07	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.575		Crippen Method
mcvol	79.370	ml/mol	McGowan Method
pc	5990.66	kPa	Joback Method
tb	330.37	K	Joback Method
tc	502.08	K	Joback Method
tf	180.78	K	Joback Method
vc	0.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.85	J/mol×K	444.84	Joback Method
cpg	144.75	J/mol×K	473.46	Joback Method
cpg	118.73	J/mol×K	330.37	Joback Method

cpg	124.23	J/mol×K	358.99	Joback Method
cpg	129.58	J/mol×K	387.61	Joback Method
cpg	134.79	J/mol×K	416.22	Joback Method
cpg	149.49	J/mol×K	502.08	Joback Method
hvapt	47.70	kJ/mol	399.00	NIST Webbook
hvapt	56.40	kJ/mol	248.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64554e+01
Coeff. B	-5.03684e+03
Coeff. C	-2.29760e+01
Temperature range (K), min.	334.51
Temperature range (K), max.	474.96

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=C594445&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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