Ethyl benzenesulfonate

Other names:	Benzenesulfonic acid ethyl ester
	Ethyl benzensulfonate
	ethyl benzenesulphonate
Inchi:	InChI=1S/C8H10O3S/c1-2-11-12(9,10)8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	XDRMBCMMABGNMM-UHFFFAOYSA-N
Formula:	C8H10O3S
SMILES:	CCOS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	186.23
CAS:	515-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-444.65	kJ/mol	Joback Method
hf	-557.49	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	56.72	kJ/mol	Joback Method
log10ws	-2.13		Aqueous Solubility Prediction Method
logp	1.412		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	479.32	K	Joback Method
tc	681.53	K	Joback Method
tf	267.13	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.51	J/mol×K	479.32	Joback Method
cpg	285.48	J/mol×K	513.02	Joback Method
cpg	297.83	J/mol×K	546.72	Joback Method
cpg	309.53	J/mol×K	580.42	Joback Method
cpg	320.60	J/mol×K	614.12	Joback Method

cpg	331.03	J/mol×K	647.82	Joback Method
cpg	340.82	J/mol×K	681.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.00	K	2.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C515468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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