

Ethanesulfonic acid

Inchi:	InChI=1S/C2H6O3S/c1-2-6(3,4)5/h2H2,1H3,(H,3,4,5)
InchiKey:	CCIVGXIOQKPBKL-UHFFFAOYSA-N
Formula:	C2H6O3S
SMILES:	CCS(=O)(=O)O
Mol. weight [g/mol]:	110.13
CAS:	594-45-6

Physical Properties

Property code	Value	Unit	Source
hf	-564.57	kJ/mol	Cheméo Relay (1.0)
hfus	16.40	kJ/mol	Joback Method
hvap	83.82	kJ/mol	Cheméo Relay (1.0)
ie	11.33	eV	Cheméo Relay (1.0)
log10ws	1.00		Cheméo Relay (1.0)
logp	-0.106		Crippen Method
mcvol	73.000	ml/mol	McGowan Method
tf	397.98	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	3.96010e+01
Coeff. B	2.61410e-01
Coeff. C	-4.98000e-05
Coeff. D	-4.08000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	srf
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	N/m
Coeff. A	6.82476e-02
Coeff. B	-8.24000e-05
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Temperature range (K), min.	256.15
Temperature range (K), max.	396.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jasper (1972), surface tension of pure liquid compounds:	https://doi.org/10.1063/1.3253106
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
srf:	Surface Tension
tf:	Normal melting (fusion) point

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