3-(Ethylsulphonyl)-1-propene

Inchi: InChI=1S/C5H10O2S/c1-3-5-8(6,7)4-2/h3H,1,4-5H2,2H3
InchiKey: QVPMTBXAMZJINK-UHFFFAOYSA-N
Formula: C5H10O2S
SMILES: C=CCS(=O)(=O)CC
Mol. weight [g/mol]: 134.20
CAS: 34008-91-8

Physical Properties

Property code	Value	Unit	Source
chl	-3593.10 ± 0.84	kJ/mol	NIST Webbook
gf	-389.48	kJ/mol	Joback Method
hf	-322.30 ± 2.70	kJ/mol	NIST Webbook
hfl	-406.00 ± 1.00	kJ/mol	NIST Webbook
hfus	18.80	kJ/mol	Joback Method
hvap	83.70 ± 2.50	kJ/mol	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.607		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
tb	358.26	K	Joback Method
tc	524.60	K	Joback Method
tf	182.91	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.74	J/mol×K	358.26	Joback Method
cpg	188.18	J/mol×K	385.98	Joback Method
cpg	197.31	J/mol×K	413.71	Joback Method
cpg	206.13	J/mol×K	441.43	Joback Method
cpg	214.63	J/mol×K	469.15	Joback Method
cpg	222.83	J/mol×K	496.87	Joback Method
cpg	230.72	J/mol×K	524.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C34008918&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume