

1,1-Bis(ethylsulfonyl) ethylene

Inchi:	InChI=1S/C6H12O4S2/c1-4-11(7,8)6(3)12(9,10)5-2/h3-5H2,1-2H3
InchiKey:	PHZCUPLOMWYPET-UHFFFAOYSA-N
Formula:	C6H12O4S2
SMILES:	<chem>C=C(S(=O)(=O)CC)S(=O)(=O)CC</chem>
Mol. weight [g/mol]:	212.29
CAS:	114223-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-858.15	kJ/mol	Joback Method
hf	-958.23	kJ/mol	Joback Method
hfus	31.46	kJ/mol	Joback Method
hvap	65.63	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.327		Crippen Method
mcvol	147.280	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	428.80	K	Joback Method
tc	596.26	K	Joback Method
tf	218.78	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.63	J/molxK	428.80	Joback Method
cpg	299.33	J/molxK	456.71	Joback Method
cpg	310.62	J/molxK	484.62	Joback Method
cpg	321.50	J/molxK	512.53	Joback Method
cpg	331.96	J/molxK	540.44	Joback Method
cpg	342.00	J/molxK	568.35	Joback Method
cpg	351.60	J/molxK	596.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C114223302&Units=SI

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
mccvol:	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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