2-Butene-1,4-disulfonic acid, dimethyl ester (cis and trans)

Inchi: InChI=1S/C6H12O6S2/c1-13(7,8)11-5-3-4-6-12-14(2,9)10/h3-4H,5-6H2,1-2H3/b4-3+
InchiKey: ROPXCSBPIJQJTK-ONEGZZNKSA-N
Formula: C6H12O6S2
SMILES: CS(=O)(=O)OCC=CCOS(C)(=O)=O
Mol. weight [g/mol]: 244.29
CAS: 70886-56-5

Physical Properties

Property code	Value	Unit	Source
gf	-1067.22	kJ/mol	Joback Method
hf	-1221.09	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-0.01		Crippen Method
logp	-0.505		Crippen Method
mcvol	159.020	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	481.24	K	Joback Method
tc	649.82	K	Joback Method
tf	273.88	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.01	J/mol×K	481.24	Joback Method
cpg	347.45	J/mol×K	509.34	Joback Method
cpg	358.53	J/mol×K	537.43	Joback Method
cpg	369.23	J/mol×K	565.53	Joback Method
cpg	379.54	J/mol×K	593.63	Joback Method
cpg	389.43	J/mol×K	621.72	Joback Method
cpg	398.89	J/mol×K	649.82	Joback Method

Sources

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=C70886565&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume