2,2-Bis(ethylsulfonyl)propane

Other names:	Propane, 2,2-bis(ethylsulfonyl)-
	Acetone diethyl sulfone
	Acetone, bis(ethyl sulfone)
	Diethylsulfondimethylmethane
	Propanediethyl sulfone
	Sulfonal
	Sulfonmethane
	Sulphonal
	2-Propanone, bis(ethyl sulfone)
	2,2-Bis(ethylsulphonyl)-propane
	NSC 26248
Inchi:	InChI=1S/C7H16O4S2/c1-5-12(8,9)7(3,4)13(10,11)6-2/h5-6H2,1-4H3
InchiKey:	CESKLHVYGRFMFP-UHFFFAOYSA-N
Formula:	C7H16O4S2
SMILES:	CCS(=O)(=O)C(C)(C)S(=O)(=O)CC
Mol. weight [g/mol]:	228.33
CAS:	115-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-926.18	kJ/mol	Joback Method
hf	-1103.26	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.592		Crippen Method
mcvol	165.670	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	451.89	K	Joback Method
tc	622.06	K	Joback Method
tf	248.19	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.43	J/mol×K	451.89	Joback Method
cpg	362.69	J/mol×K	480.25	Joback Method
cpg	376.35	J/mol×K	508.61	Joback Method
cpg	389.41	J/mol×K	536.97	Joback Method
cpg	401.88	J/mol×K	565.33	Joback Method
cpg	413.75	J/mol×K	593.69	Joback Method
cpg	425.04	J/mol×K	622.06	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=C115242&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume