1,3-dithietane

Other names: 1,3-Dithiethane
Inchi: InChI=1S/C2H4S2/c1-3-2-4-1/h1-2H2
InchiKey: ITXACGPMGJCSKF-UHFFFAOYSA-N
Formula: C2H4S2
SMILES: C1SCS1
Mol. weight [g/mol]: 92.18
CAS: 287-53-6

Physical Properties

Property code	Value	Unit	Source
gf	102.04	kJ/mol	Joback Method
hf	92.89	kJ/mol	Joback Method
hfus	3.21	kJ/mol	Joback Method
hvap	32.06	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.381		Crippen Method
mcvol	60.880	ml/mol	McGowan Method
pc	6567.04	kPa	Joback Method
rinpol	806.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	806.00		NIST Webbook
tb	356.50	K	Joback Method
tc	587.90	K	Joback Method
tf	297.86	K	Joback Method
vc	0.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	83.70	J/mol×K	356.50	Joback Method
cpg	90.66	J/mol×K	395.07	Joback Method
cpg	97.02	J/mol×K	433.63	Joback Method
cpg	102.82	J/mol×K	472.20	Joback Method
cpg	108.13	J/mol×K	510.76	Joback Method
cpg	112.96	J/mol×K	549.33	Joback Method
cpg	117.38	J/mol×K	587.90	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=C287536&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
ie: Ionization energy
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