1,3-Dithiolane

Other names: 1,3-Dithiacyclopentane
Inchi: InChI=1S/C3H6S2/c1-2-5-3-4-1/h1-3H2
InchiKey: IMLSAISZLJGWPP-UHFFFAOYSA-N
Formula: C3H6S2
SMILES: C1CSCS1
Mol. weight [g/mol]: 106.21
CAS: 4829-04-3

Physical Properties

Property code	Value	Unit	Source
gf	98.36	kJ/mol	Joback Method
hf	66.09	kJ/mol	Joback Method
hfus	3.70	kJ/mol	Joback Method
hvap	34.46	kJ/mol	Joback Method
ie	8.75	eV	NIST Webbook
ie	8.77	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-1.24		Crippen Method
logp	1.424		Crippen Method
mcvol	74.970	ml/mol	McGowan Method
pc	5871.90	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	978.00		NIST Webbook
tb	448.20	K	NIST Webbook
tc	623.34	K	Joback Method
tf	305.61	K	Joback Method
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.20	J/mol×K	383.65	Joback Method
cpg	122.76	J/mol×K	423.60	Joback Method
cpg	131.61	J/mol×K	463.55	Joback Method
cpg	139.81	J/mol×K	503.50	Joback Method
cpg	147.38	J/mol×K	543.44	Joback Method
cpg	154.38	J/mol×K	583.39	Joback Method
cpg	160.85	J/mol×K	623.34	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=C4829043&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