

1,3-Dithiolan-2-one

Other names:	1,3-Dithiacyclopentane-2-one
Inchi:	InChI=1S/C3H4OS2/c4-3-5-1-2-6-3/h1-2H2
InchiKey:	ZBEWVJOWXJNDGJ-UHFFFAOYSA-N
Formula:	C3H4OS2
SMILES:	O=C1SCCS1
Mol. weight [g/mol]:	120.19
CAS:	2080-58-2

Physical Properties

Property code	Value	Unit	Source
chs	-2751.00 ± 5.00	kJ/mol	NIST Webbook
gf	-24.23	kJ/mol	Joback Method
hf	-125.90 ± 5.10	kJ/mol	NIST Webbook
hfus	3.21	kJ/mol	Joback Method
hsub	80.30 ± 0.40	kJ/mol	NIST Webbook
hvap	38.71	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.58	eV	NIST Webbook
log10ws	-1.49		Crippen Method
logp	1.586		Crippen Method
mcvol	76.540	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
tb	451.47	K	Joback Method
tc	714.75	K	Joback Method
tf	373.83	K	Joback Method
vc	0.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.79	J/molxK	451.47	Joback Method
cpg	137.39	J/molxK	495.35	Joback Method
cpg	145.52	J/molxK	539.23	Joback Method
cpg	153.19	J/molxK	583.11	Joback Method

cpg	160.39	J/mol×K	626.99	Joback Method
cpg	167.12	J/mol×K	670.87	Joback Method
cpg	173.39	J/mol×K	714.75	Joback Method

Sources

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=C2080582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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