

1,2-Dithian-4-one

Inchi:	InChI=1S/C4H6OS2/c5-4-1-2-6-7-3-4/h1-3H2
InchiKey:	KEYSLSNDOHVVSK-UHFFFAOYSA-N
Formula:	C4H6OS2
SMILES:	O=C1CCSSC1
Mol. weight [g/mol]:	134.22

Physical Properties

Property code	Value	Unit	Source
gf	-27.91	kJ/mol	Joback Method
hf	-98.41	kJ/mol	Joback Method
hfus	3.70	kJ/mol	Joback Method
hvap	41.11	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.341		Crippen Method
mcvol	90.630	ml/mol	McGowan Method
pc	5560.87	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
tb	478.62	K	Joback Method
tc	747.66	K	Joback Method
tf	381.58	K	Joback Method
vc	0.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.20	J/mol×K	478.62	Joback Method
cpg	176.55	J/mol×K	523.46	Joback Method
cpg	187.27	J/mol×K	568.30	Joback Method
cpg	197.34	J/mol×K	613.14	Joback Method
cpg	206.76	J/mol×K	657.98	Joback Method
cpg	215.52	J/mol×K	702.82	Joback Method
cpg	223.60	J/mol×K	747.66	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=R227602&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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