

2,3,5,7-tetrathiaoctane

Inchi:	InChI=1S/C4H10S4/c1-5-3-7-4-8-6-2/h3-4H2,1-2H3
InchiKey:	FFPNIJFTQRBINC-UHFFFAOYSA-N
Formula:	C4H10S4
SMILES:	CSCSCSSC
Mol. weight [g/mol]:	186.38

Physical Properties

Property code	Value	Unit	Source
gf	115.28	kJ/mol	Joback Method
hf	41.59	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	51.77	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.009		Crippen Method
mcvol	132.620	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	1464.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	566.04	K	Joback Method
tc	831.53	K	Joback Method
tf	272.44	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.22	J/mol×K	566.04	Joback Method
cpg	269.10	J/mol×K	610.29	Joback Method
cpg	279.31	J/mol×K	654.54	Joback Method
cpg	288.83	J/mol×K	698.79	Joback Method
cpg	297.61	J/mol×K	743.03	Joback Method
cpg	305.61	J/mol×K	787.28	Joback Method
cpg	312.80	J/mol×K	831.53	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=R226387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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