

# Nonane, 3,4-bis-(methylthio), erythro

<b>Inchi:</b>	InChI=1S/C11H24S2/c1-5-7-8-9-11(13-4)10(6-2)12-3/h10-11H,5-9H2,1-4H3/t10-,11+/m1
<b>InchiKey:</b>	QOQHJDISUURNU-MNOVXSKESA-N
<b>Formula:</b>	C11H24S2
<b>SMILES:</b>	CCCCC(SC)C(CC)SC
<b>Mol. weight [g/mol]:</b>	220.44

## Physical Properties

Property code	Value	Unit	Source
gf	103.10	kJ/mol	Joback Method
hf	-197.19	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.440		Crippen Method
mvol	198.550	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rmpol	1552.00		NIST Webbook
tb	587.76	K	Joback Method
tc	793.00	K	Joback Method
tf	252.53	K	Joback Method
vc	0.748	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.51	J/mol×K	587.76	Joback Method
cpg	503.08	J/mol×K	621.97	Joback Method
cpg	519.75	J/mol×K	656.17	Joback Method
cpg	535.55	J/mol×K	690.38	Joback Method
cpg	550.48	J/mol×K	724.59	Joback Method
cpg	564.56	J/mol×K	758.80	Joback Method
cpg	577.81	J/mol×K	793.00	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R121816&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R121816&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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