

# 1-Naphthalenecarbothioic acid, O-ethyl ester

<b>Inchi:</b>	InChI=1S/C13H12OS/c1-2-14-13(15)12-9-5-7-10-6-3-4-8-11(10)12/h3-9H,2H2,1H3
<b>InchiKey:</b>	IMSIYJBXAHWVMY-UHFFFAOYSA-N
<b>Formula:</b>	C13H12OS
<b>SMILES:</b>	CCOC(=S)c1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	216.30
<b>CAS:</b>	58303-26-7

## Physical Properties

Property code	Value	Unit	Source
gf	280.07	kJ/mol	Joback Method
hf	118.76	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.552		Crippen Method
mcvol	168.730	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	639.94	K	Joback Method
tc	887.02	K	Joback Method
tf	364.41	K	Joback Method
vc	0.631	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.32	J/molxK	639.94	Joback Method
cpg	412.10	J/molxK	681.12	Joback Method
cpg	424.80	J/molxK	722.30	Joback Method
cpg	436.54	J/molxK	763.48	Joback Method
cpg	447.43	J/molxK	804.66	Joback Method
cpg	457.58	J/molxK	845.84	Joback Method
cpg	467.12	J/molxK	887.02	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=C58303267&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58303267&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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