

# Phenylthioacetamide, N,N-dinonyl-

**Inchi:** InChI=1S/C26H45NOS/c1-3-5-7-9-11-13-18-22-27(23-19-14-12-10-8-6-4-2)26(28)24-29-  
**InchiKey:** UVWOPRXNFHKUBZ-UHFFFAOYSA-N  
**Formula:** C26H45NOS  
**SMILES:** CCCCCCCCCN(CCCCCCCC)C(=O)CSc1ccccc1  
**Mol. weight [g/mol]:** 419.71

## Physical Properties

Property code	Value	Unit	Source
gf	295.43	kJ/mol	Joback Method
hf	-346.62	kJ/mol	Joback Method
hfus	65.89	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	8.108		Crippen Method
mvol	381.340	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	3288.00		NIST Webbook
rinpol	3288.00		NIST Webbook
tb	956.05	K	Joback Method
tc	1170.64	K	Joback Method
tf	526.00	K	Joback Method
vc	1.462	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.50	J/molxK	956.05	Joback Method
cpg	1291.62	J/molxK	991.82	Joback Method
cpg	1309.43	J/molxK	1027.58	Joback Method
cpg	1326.03	J/molxK	1063.35	Joback Method
cpg	1341.50	J/molxK	1099.11	Joback Method
cpg	1355.93	J/molxK	1134.88	Joback Method
cpg	1369.42	J/molxK	1170.64	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<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=U308166&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308166&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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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