

# (E) 1-Phenylthio-1-butene

<b>Inchi:</b>	InChI=1S/C10H12S/c1-2-3-9-11-10-7-5-4-6-8-10/h3-9H,2H2,1H3/b9-3+
<b>InchiKey:</b>	PXAUEKOLGHSMRX-YCRREMRBSA-N
<b>Formula:</b>	C10H12S
<b>SMILES:</b>	CCC=CSc1ccccc1
<b>Mol. weight [g/mol]:</b>	164.27
<b>CAS:</b>	21106-26-3

## Physical Properties

Property code	Value	Unit	Source
gf	259.07	kJ/mol	Joback Method
hf	145.89	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.702		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	527.82	K	Joback Method
tc	765.27	K	Joback Method
tf	258.20	K	Joback Method
vc	0.521	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.46	J/mol×K	527.82	Joback Method
cpg	306.31	J/mol×K	567.40	Joback Method
cpg	320.13	J/mol×K	606.97	Joback Method
cpg	332.95	J/mol×K	646.55	Joback Method
cpg	344.83	J/mol×K	686.12	Joback Method
cpg	355.84	J/mol×K	725.70	Joback Method
cpg	366.03	J/mol×K	765.27	Joback Method

# Sources

<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>
<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=C21106263&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21106263&amp;Units=SI</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>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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