Thiourea, (phenylmethyl)-

Other names:	Benzylthiourea
	Urea, 1-benzyl-2-thio-
Inchi:	InChI=1S/C8H10N2S/c9-8(11)10-6-7-4-2-1-3-5-7/h1-5H,6H2,(H3,9,10,11)
InchiKey:	UCGFRIAOVLXVKL-UHFFFAOYSA-N
Formula:	C8H10N2S
SMILES:	NC(=S)NCc1ccccc1
Mol. weight [g/mol]:	166.24
CAS:	621-83-0

Physical Properties

Property code	Value	Unit	Source
gf	401.79	kJ/mol	Joback Method
hf	261.84	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	59.48	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.020		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	601.86	K	Joback Method
tc	850.91	K	Joback Method
tf	376.53	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.92	J/mol×K	601.86	Joback Method
cpg	312.45	J/mol×K	643.37	Joback Method
cpg	322.98	J/mol×K	684.88	Joback Method
cpg	332.63	J/mol×K	726.39	Joback Method
cpg	341.49	J/mol×K	767.89	Joback Method
cpg	349.67	J/mol×K	809.40	Joback Method
cpg	357.26	J/mol×K	850.91	Joback Method

Sources

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=C621830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume