Thiourea, N-phenyl-N'-(phenylmethyl)-

Other names: Urea, 1-benzyl-3-phenyl-2-thio-
N-Phenyl-N'-benzylthiourea
1-Benzyl-3-phenylthiourea
Inchi: InChI=1S/C14H14N2S/c17-14(16-13-9-5-2-6-10-13)15-11-12-7-3-1-4-8-12/h1-10H,11H2
InchiKey: NXCBDDGSOXJEFZ-UHFFFAOYSA-N
Formula: C14H14N2S
SMILES: S=C(NCc1ccccc1)Nc1ccccc1
Mol. weight [g/mol]: 242.34
CAS: 726-25-0

Physical Properties

Property code	Value	Unit	Source
gf	587.66	kJ/mol	Joback Method
hf	394.21	kJ/mol	Joback Method
hfus	34.90	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.173		Crippen Method
mcvol	192.610	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	743.46	K	Joback Method
tc	999.69	K	Joback Method
tf	439.97	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.13	J/mol×K	743.46	Joback Method
cpg	518.05	J/mol×K	786.17	Joback Method
cpg	530.79	J/mol×K	828.87	Joback Method
cpg	542.52	J/mol×K	871.58	Joback Method
cpg	553.38	J/mol×K	914.28	Joback Method
cpg	563.55	J/mol×K	956.99	Joback Method

cpg	573.16	J/mol×K	999.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C726250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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