Methanethione, diphenyl-

Other names:	Benzothione
	Benzothiophenone
	Thiobenzophenone
Inchi:	InChI=1S/C13H10S/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H
InchiKey:	XDDVRYDDMGRFAZ-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	S=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	198.28
CAS:	1450-31-3

Physical Properties

Property code	Value	Unit	Source
gf	400.46	kJ/mol	Joback Method
hf	307.91	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.453		Crippen Method
mcvol	158.560	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
tb	620.24	K	Joback Method
tc	891.80	K	Joback Method
tf	323.38	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.34	J/mol×K	620.24	Joback Method
cpg	371.33	J/mol×K	665.50	Joback Method
cpg	384.85	J/mol×K	710.76	Joback Method
cpg	397.08	J/mol×K	756.02	Joback Method

cpg	408.19	J/mol×K	801.28	Joback Method
cpg	418.33	J/mol×K	846.54	Joback Method
cpg	427.69	J/mol×K	891.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1450313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume