Disulfide, diphenyl

Other names:	Phenyl disulfide
	Diphenyl disulfide
	USAF e-1
	diphenyl disulphide
Inchi:	InChI=1S/C12H10S2/c1-3-7-11(8-4-1)13-14-12-9-5-2-6-10-12/h1-10H
InchiKey:	GUUVPOWQJOLRAS-UHFFFAOYSA-N
Formula:	C12H10S2
SMILES:	c1ccc(SSc2ccccc2)cc1
Mol. weight [g/mol]:	218.34
CAS:	882-33-7

Physical Properties

Property code	Value	Unit	Source
chs	-7504.40 ± 2.70	kJ/mol	NIST Webbook
chs	-7503.18	kJ/mol	NIST Webbook
gf	341.22	kJ/mol	Joback Method
hf	244.00 ± 4.20	kJ/mol	NIST Webbook
hf	246.00	kJ/mol	NIST Webbook
hfs	151.06	kJ/mol	NIST Webbook
hfs	149.10 ± 2.70	kJ/mol	NIST Webbook
hfus	23.18	kJ/mol	Joback Method
hsub	95.00 ± 2.00	kJ/mol	NIST Webbook
hsub	94.90	kJ/mol	NIST Webbook
hvap	78.70 ± 2.90	kJ/mol	NIST Webbook
ie	9.40 ± 0.30	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-4.76		Crippen Method
logp	4.486		Crippen Method
mcvol	165.120	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	664.88	K	Joback Method
tc	955.79	K	Joback Method
tf	333.50 ± 1.00	K	NIST Webbook
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.57	J/mol×K	858.82	Joback Method
cpg	439.97	J/mol×K	907.31	Joback Method
cpg	378.83	J/mol×K	664.88	Joback Method
cpg	394.06	J/mol×K	713.37	Joback Method
cpg	407.71	J/mol×K	761.85	Joback Method
cpg	419.85	J/mol×K	810.34	Joback Method
cpg	448.12	J/mol×K	955.79	Joback Method
hvapt	72.40	kJ/mol	494.00	NIST Webbook
hvapt	74.40	kJ/mol	493.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C882337&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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