Disulfide, bis(phenylmethyl)

Other names:	1,4-diphenyl-2,3-dithiabutane
	BDS
	Benzyl bisulfide
	Benzyl disulfide
	Bis(phenylmethyl) disulfide
	Di(phenylmethyl)disulfide
	Dibenzyl disulphide
	Dibenzyldisulfid
	Disulfide, dibenzyl
	NSC 677465
	NSC 6841
	dibenzyl disulfide
	«alpha»-(Benzyldithio)toluene
Inchi:	InChI=1S/C14H14S2/c1-3-7-13(8-4-1)11-15-16-12-14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey:	GVPWHKZIJBODOX-UHFFFAOYSA-N
Formula:	C14H14S2
SMILES:	c1ccc(CSSCc2ccccc2)cc1
Mol. weight [g/mol]:	246.39
CAS:	150-60-7

Physical Properties

Property code	Value	Unit	Source
gf	358.06	kJ/mol	Joback Method
hf	224.51	kJ/mol	Joback Method
hfus	44.97	kJ/mol	Heat capacity and thermodynamic properties of benzyl disulfide (C14H14S2)
hvap	64.94	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.768		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	2070.00		NIST Webbook
tb	710.64	K	Joback Method
tc	986.29	K	Joback Method
tf	342.00 ± 2.00	K	NIST Webbook
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.05	J/mol×K	710.64	Joback Method
cpg	496.26	J/mol×K	756.58	Joback Method
cpg	510.88	J/mol×K	802.52	Joback Method
cpg	524.00	J/mol×K	848.46	Joback Method
cpg	535.71	J/mol×K	894.40	Joback Method
cpg	546.09	J/mol×K	940.35	Joback Method
cpg	555.23	J/mol×K	986.29	Joback Method
hfust	44.70	kJ/mol	341.70	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat capacity and thermodynamic properties of benzyl disulfide (C14H14S2).	https://www.doi.org/10.1016/j.tca.2007.05.014
Solubility of Benzyl Disulfide in Five Organic Solvents between (283.45 and 333.15) K.	https://www.doi.org/10.1021/je400326r
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=C150607&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
hfust:	Enthalpy of fusion at a given temperature
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