Bitoscanate

Other names:	Benzene, 1,4-diisothiocyanato-
	Isothiocyanic acid, p-phenylene ester
	p-Phenylene bis(isothiocyanate)
	p-Phenylene diisothiocyanate
	Bitoscanat
	Jonit
	Phenylene 1,4-diisothiocyanate
	WM 842
	1,4-Diisothiocyanatobenzene
	1,4-Phenylene diisothiocyanate
	Isothiocyanic acid, 1,4-phenylenedi-
	Biscomate
Inchi:	InChI=1S/C8H4N2S2/c11-5-9-7-1-2-8(4-3-7)10-6-12/h1-4H
InchiKey:	OMWQUXGVXQELIX-UHFFFAOYSA-N
Formula:	C8H4N2S2
SMILES:	S=C=Nc1ccc(N=C=S)cc1
Mol. weight [g/mol]:	192.26
CAS:	4044-65-9

Physical Properties

Property code	Value	Unit	Source
hf	584.75	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.155		Crippen Method
mcvol	135.280	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	706.00	K	Joback Method
tc	1007.91	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4044659&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

hf:	Enthalpy of formation 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