1,3-Benzodithiole,2-(1,3-benzodithiol-2-ylidene)-

Inchi: InChI=1S/C14H8S4/c1-2-6-10-9(5-1)15-13(16-10)14-17-11-7-3-4-8-12(11)18-14/h1-8H
InchiKey: OVIRUXIWCFZJQC-UHFFFAOYSA-N
Formula: C14H8S4
SMILES: c1ccc2c(c1)SC(=C1Sc3ccccc3S1)S2
Mol. weight [g/mol]: 304.47
CAS: 24648-13-3

Physical Properties

Property code	Value	Unit	Source
gf	579.62	kJ/mol	Joback Method
hf	519.99	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	77.94	kJ/mol	Joback Method
ie	6.81	eV	NIST Webbook
ie	6.68	eV	NIST Webbook
log10ws	-6.88		Crippen Method
logp	5.909		Crippen Method
mcvol	199.980	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	806.30	K	Joback Method
tc	1132.20	K	Joback Method
tf	729.38	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.67	J/mol×K	806.30	Joback Method
cpg	483.71	J/mol×K	860.62	Joback Method
cpg	495.10	J/mol×K	914.93	Joback Method
cpg	506.24	J/mol×K	969.25	Joback Method
cpg	517.50	J/mol×K	1023.57	Joback Method
cpg	529.27	J/mol×K	1077.88	Joback Method
cpg	541.93	J/mol×K	1132.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24648133&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

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
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