1,3-Benzenedithiol

Other names:	Benzene-1,3-dithiol
	1,3-Benzedithiol
Inchi:	InChI=1S/C6H6S2/c7-5-2-1-3-6(8)4-5/h1-4,7-8H
InchiKey:	ZWOASCVFHSYHOB-UHFFFAOYSA-N
Formula:	C6H6S2
SMILES:	Sc1cccc(S)c1
Mol. weight [g/mol]:	142.24
CAS:	626-04-0

Physical Properties

Property code	Value	Unit	Source
gf	161.20	kJ/mol	Joback Method
hf	134.85	kJ/mol	Joback Method
hfus	13.03	kJ/mol	Joback Method
hvap	45.36	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.264		Crippen Method
mcvol	104.340	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
ripol	2467.00		NIST Webbook
ripol	2467.00		NIST Webbook
tb	518.00	K	NIST Webbook
tb	518.20	K	NIST Webbook
tc	766.38	K	Joback Method
tf	300.00	K	NIST Webbook
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.33	J/mol×K	494.06	Joback Method
cpg	192.58	J/mol×K	539.45	Joback Method
cpg	202.02	J/mol×K	584.83	Joback Method
cpg	210.70	J/mol×K	630.22	Joback Method

cpg	218.65	J/mol×K	675.61	Joback Method
cpg	225.92	J/mol×K	721.00	Joback Method
cpg	232.55	J/mol×K	766.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.70	K	2.10	NIST Webbook
tbrp	335.00	K	0.03	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626040&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume