

1,2-Benzenedithiol

Other names:	Benzene-1,2-dithiol
Inchi:	InChI=1S/C6H6S2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H
InchiKey:	JRNVQLOKVMWBFR-UHFFFAOYSA-N
Formula:	C6H6S2
SMILES:	Sc1ccccc1S
Mol. weight [g/mol]:	142.24
CAS:	17534-15-5

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
tb	511.50 ± 0.50	K	NIST Webbook
tb	511.70	K	NIST Webbook
tc	766.38	K	Joback Method
tf	300.50 ± 0.50	K	NIST Webbook
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.33	J/molxK	494.06	Joback Method
cpg	192.58	J/molxK	539.45	Joback Method
cpg	202.02	J/molxK	584.83	Joback Method
cpg	210.70	J/molxK	630.22	Joback Method
cpg	218.65	J/molxK	675.61	Joback Method
cpg	225.92	J/molxK	721.00	Joback Method
cpg	232.55	J/molxK	766.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	2.30	NIST Webbook
tbrp	333.50 ± 0.50	K	0.01	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C17534155&Units=SI

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

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