

1,4-Benzenedithiol

Other names:	«alpha», «alpha»'-p-Xylenedithiol p-Xylene-«alpha», «alpha»'-dithiol p-Xylylenedithiol 1,4-Benzenebis(methanethiol) 1,4-Bis(mercaptomethyl)benzene 4-(Sulfanylmethyl)benzyl hydrosulfide
Inchi:	InChI=1S/C8H10S2/c9-5-7-1-2-8(6-10)4-3-7/h1-4,9-10H,5-6H2
InchiKey:	IYPNRTQAOXLCQW-UHFFFAOYSA-N
Formula:	C8H10S2
SMILES:	SCc1ccc(CS)cc1
Mol. weight [g/mol]:	170.29
CAS:	105-09-9

Physical Properties

Property code	Value	Unit	Source
gf	178.04	kJ/mol	Joback Method
hf	93.57	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	49.81	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.546		Crippen Method
mvol	132.520	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	1578.80		NIST Webbook
tb	539.82	K	Joback Method
tc	800.21	K	Joback Method
tf	319.50 ± 0.50	K	NIST Webbook
vc	0.483	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.44	J/mol×K	539.82	Joback Method
cpg	278.40	J/mol×K	583.22	Joback Method

cpg	290.41	J/mol×K	626.62	Joback Method
cpg	301.51	J/mol×K	670.01	Joback Method
cpg	311.75	J/mol×K	713.41	Joback Method
cpg	321.18	J/mol×K	756.81	Joback Method
cpg	329.85	J/mol×K	800.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.00	K	1.60	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=C105099&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
rinpol:	Non-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

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