m-Xylene-«alpha»,«alpha»'-dithiol

Other names: 1,3-Benzenedimethanethiol
3-(Sulfanylmethyl)benzyl hydrosulfide
Inchi: InChI=1S/C8H10S2/c9-5-7-2-1-3-8(4-7)6-10/h1-4,9-10H,5-6H2
InchiKey: JSNABGZJVWSNOB-UHFFFAOYSA-N
Formula: C8H10S2
SMILES: SCc1cccc(CS)c1
Mol. weight [g/mol]: 170.29
CAS: 41563-69-3

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
mcvol	132.520	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	1561.30		NIST Webbook
rinpol	1561.30		NIST Webbook
tb	539.82	K	Joback Method
tc	800.21	K	Joback Method
tf	291.78	K	Joback Method
vc	0.483	m3/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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41563693&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume