1,2-Benzenedimethanethiol, S-acetyl-

Inchi: InChI=1S/C10H12OS2/c1-8(11)13-7-10-5-3-2-4-9(10)6-12/h2-5,12H,6-7H2,1H3
InchiKey: NMWYBJAAZOILGV-UHFFFAOYSA-N
Formula: C10H12OS2
SMILES: CC(=O)SCc1ccccc1CS
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	69.69	kJ/mol	Joback Method
hf	-56.90	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	61.09	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.896		Crippen Method
mcvol	162.270	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1774.80		NIST Webbook
rinpol	1774.80		NIST Webbook
tb	645.37	K	Joback Method
tc	900.32	K	Joback Method
tf	362.19	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.48	J/mol×K	645.37	Joback Method
cpg	385.87	J/mol×K	687.86	Joback Method
cpg	398.22	J/mol×K	730.35	Joback Method
cpg	409.57	J/mol×K	772.84	Joback Method
cpg	419.94	J/mol×K	815.34	Joback Method
cpg	429.39	J/mol×K	857.83	Joback Method
cpg	437.93	J/mol×K	900.32	Joback Method

Sources

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=U353028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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