1,2-Benzenedithiol, S,S'-diacetyl-

Inchi: InChI=1S/C10H10O2S2/c1-7(11)13-9-5-3-4-6-10(9)14-8(2)12/h3-6H,1-2H3
InchiKey: GDKGFYKZMCDPDM-UHFFFAOYSA-N
Formula: C10H10O2S2
SMILES: CC(=O)Sc1ccccc1SC(C)=O
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-55.50	kJ/mol	Joback Method
hf	-166.09	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.964		Crippen Method
mcvol	163.840	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	1788.60		NIST Webbook
rinpol	1788.60		NIST Webbook
tb	705.16	K	Joback Method
tc	964.78	K	Joback Method
tf	410.06	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.77	J/mol×K	705.16	Joback Method
cpg	397.50	J/mol×K	748.43	Joback Method
cpg	408.15	J/mol×K	791.70	Joback Method
cpg	417.74	J/mol×K	834.97	Joback Method
cpg	426.29	J/mol×K	878.24	Joback Method
cpg	433.81	J/mol×K	921.51	Joback Method
cpg	440.32	J/mol×K	964.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353063&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume