1,2-Benzenedimethanethiol, S,S'-diacetyl-

Inchi: InChI=1S/C12H14O2S2/c1-9(13)15-7-11-5-3-4-6-12(11)8-16-10(2)14/h3-6H,7-8H2,1-2H
InchiKey: QWQXTHVGDKJKJU-UHFFFAOYSA-N
Formula: C12H14O2S2
SMILES: CC(=O)SCc1ccccc1CSC(C)=O
Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
gf	-38.66	kJ/mol	Joback Method
hf	-207.37	kJ/mol	Joback Method
hfus	31.95	kJ/mol	Joback Method
hvap	72.37	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.246		Crippen Method
mcvol	192.020	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	2010.50		NIST Webbook
rinpol	2010.50		NIST Webbook
tb	750.92	K	Joback Method
tc	999.06	K	Joback Method
tf	432.60	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.72	J/mol×K	750.92	Joback Method
cpg	500.54	J/mol×K	792.28	Joback Method
cpg	512.21	J/mol×K	833.63	Joback Method
cpg	522.76	J/mol×K	874.99	Joback Method
cpg	532.21	J/mol×K	916.35	Joback Method
cpg	540.59	J/mol×K	957.70	Joback Method
cpg	547.92	J/mol×K	999.06	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=U353026&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