2,4-Thiazolidinedione, 5-p-hydroxybenzylidene-

Inchi: InChI=1S/C10H7NO3S/c12-7-3-1-6(2-4-7)5-8-9(13)11-10(14)15-8/h1-5,12H,(H,11,13,14)
InchiKey: ARHIHDVVUHVQCP-VMPITWQZSA-N
Formula: C10H7NO3S
SMILES: O=C1N=C(O)C(=Cc2ccc(O)cc2)S1
Mol. weight [g/mol]: 221.23
CAS: 103788-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-1.61	kJ/mol	Joback Method
hf	-161.05	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	88.40	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.556		Crippen Method
mcvol	148.180	ml/mol	McGowan Method
pc	5800.57	kPa	Joback Method
tb	827.76	K	Joback Method
tc	1092.17	K	Joback Method
tf	663.41	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.77	J/mol×K	827.76	Joback Method
cpg	422.35	J/mol×K	871.83	Joback Method
cpg	431.17	J/mol×K	915.90	Joback Method
cpg	439.32	J/mol×K	959.97	Joback Method
cpg	446.89	J/mol×K	1004.03	Joback Method
cpg	453.95	J/mol×K	1048.10	Joback Method
cpg	460.58	J/mol×K	1092.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103788609&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume