2,4-Thiazolidinedione, 5-p-chlorobenzylidene-

Inchi: InChI=1S/C10H6ClNO2S/c11-7-3-1-6(2-4-7)5-8-9(13)12-10(14)15-8/h1-5H,(H,12,13,14)/
InchiKey: OTTGINRZTJUWBT-VMPITWQZSA-N
Formula: C10H6ClNO2S
SMILES: O=C1NC(=O)C(=Cc2ccc(Cl)cc2)S1
Mol. weight [g/mol]: 239.68
CAS: 24138-83-8

Physical Properties

Property code	Value	Unit	Source
gf	96.28	kJ/mol	Joback Method
hf	-75.89	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.664		Crippen Method
mcvol	154.550	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	755.90	K	Joback Method
tc	1050.37	K	Joback Method
tf	621.74	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.42	J/mol×K	755.90	Joback Method
cpg	384.85	J/mol×K	804.98	Joback Method
cpg	395.92	J/mol×K	854.06	Joback Method
cpg	405.60	J/mol×K	903.14	Joback Method
cpg	413.83	J/mol×K	952.22	Joback Method
cpg	420.57	J/mol×K	1001.29	Joback Method
cpg	425.77	J/mol×K	1050.37	Joback Method

Sources

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=C24138838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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