2,4-Thiazolidinedione, 5-benzylidene-

Inchi: InChI=1S/C10H7NO2S/c12-9-8(14-10(13)11-9)6-7-4-2-1-3-5-7/h1-6H,(H,11,12,13)/b8-6+
InchiKey: SGIZECXZFLAGBW-SOFGYWHQSA-N
Formula: C10H7NO2S
SMILES: O=C1NC(=O)C(=Cc2ccccc2)S1
Mol. weight [g/mol]: 205.23
CAS: 3774-99-0

Physical Properties

Property code	Value	Unit	Source
gf	117.84	kJ/mol	Joback Method
hf	-48.68	kJ/mol	Joback Method
hfus	21.15	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.010		Crippen Method
mcvol	142.310	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	713.49	K	Joback Method
tc	1006.30	K	Joback Method
tf	579.30	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.07	J/mol×K	713.49	Joback Method
cpg	367.04	J/mol×K	762.29	Joback Method
cpg	379.66	J/mol×K	811.09	Joback Method
cpg	390.89	J/mol×K	859.89	Joback Method
cpg	400.72	J/mol×K	908.69	Joback Method
cpg	409.09	J/mol×K	957.50	Joback Method
cpg	415.98	J/mol×K	1006.30	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=C3774990&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume