2,4-Thiazolidinedione, 5-(p-dimethylaminobenzylidene)-

Inchi: InChI=1S/C12H12N2O2S/c1-14(2)9-5-3-8(4-6-9)7-10-11(15)13-12(16)17-10/h3-7H,1-2H
InchiKey: FONFGNGCCZIGRM-JXMROGBWSA-N
Formula: C12H12N2O2S
SMILES: CN(C)c1ccc(C=C2SC(=O)NC2=O)cc1
Mol. weight [g/mol]: 248.30
CAS: 3695-48-5

Physical Properties

Property code	Value	Unit	Source
gf	235.83	kJ/mol	Joback Method
hf	-33.90	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.076		Crippen Method
mcvol	180.470	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	776.67	K	Joback Method
tc	1049.52	K	Joback Method
tf	646.83	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.20	J/mol×K	776.67	Joback Method
cpg	509.14	J/mol×K	822.15	Joback Method
cpg	522.60	J/mol×K	867.62	Joback Method
cpg	534.59	J/mol×K	913.10	Joback Method
cpg	545.09	J/mol×K	958.57	Joback Method
cpg	554.09	J/mol×K	1004.05	Joback Method
cpg	561.59	J/mol×K	1049.52	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=C3695485&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