Thiazolidine-2,4-dione, 5-(4-methoxyphenyl)methylene-

Other names: Thiazolidine-2,4-dione, 5-(4-methoxyphenyl)methylene-
5-(4-Methoxybenzylidene)-1,3-thiazolidine-2,4-dione
2,4-Thiazolidinedione, 5-p-methoxybenzylidene-
NSC 31205

Inchi: InChI=1S/C11H9NO3S/c1-15-8-4-2-7(3-5-8)6-9-10(13)12-11(14)16-9/h2-6H,1H3,(H,12,1

InchiKey: VRUKGUBMRBLJJW-TWGQIWQCSA-N

Formula: C11H9NO3S

SMILES: COc1ccc(/C=C2\SC(=O)NC2=O)cc1

Mol. weight [g/mol]: 235.26

Physical Properties

Property code	Value	Unit	Source
hfus	24.54	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	Cheméo Relay (1.0)
log10ws	-3.64		Cheméo Relay (1.0)
logp	2.019		Crippen Method
mcvol	162.270	ml/mol	McGowan Method
tb	638.49	K	Cheméo Relay (1.0)
tf	441.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.10	J/mol×K	763.77	Joback Method
cpg	441.06	J/mol×K	810.39	Joback Method
cpg	453.57	J/mol×K	857.00	Joback Method
cpg	464.57	J/mol×K	903.62	Joback Method
cpg	474.00	J/mol×K	950.24	Joback Method
cpg	481.77	J/mol×K	996.86	Joback Method
cpg	487.82	J/mol×K	1043.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6320510&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point