

2,4-Thiazolidinedione, 5-(m-nitrobenzylidene)-

Inchi:	InChI=1S/C10H6N2O4S/c13-9-8(17-10(14)11-9)5-6-2-1-3-7(4-6)12(15)16/h1-5H,(H,11,1
InchiKey:	HWOVMANHBOBQRW-VMPITWQZSA-N
Formula:	C10H6N2O4S
SMILES:	O=C1NC(=O)C(=Cc2ccccc([N+](=O)[O-])c2)S1
Mol. weight [g/mol]:	250.23
CAS:	24044-52-8

Physical Properties

Property code	Value	Unit	Source
gf	143.76	kJ/mol	Joback Method
hf	-70.91	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	1.919		Crippen Method
mcvol	159.730	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	870.31	K	Joback Method
tc	1177.30	K	Joback Method
tf	735.43	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.63	J/molxK	870.31	Joback Method
cpg	445.94	J/molxK	921.47	Joback Method
cpg	454.51	J/molxK	972.64	Joback Method
cpg	461.31	J/molxK	1023.80	Joback Method
cpg	466.28	J/molxK	1074.97	Joback Method
cpg	469.39	J/molxK	1126.13	Joback Method
cpg	470.60	J/molxK	1177.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C24044528&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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