

2,4-Thiazolidinedione, 5-cyclohexylidene-

Inchi:	InChI=1S/C9H11NO2S/c11-8-7(13-9(12)10-8)6-4-2-1-3-5-6/h1-5H2,(H,10,11,12)
InchiKey:	OAXPSIPBZAUIDS-UHFFFAOYSA-N
Formula:	C9H11NO2S
SMILES:	O=C1NC(=O)C(=C2CCCCC2)S1
Mol. weight [g/mol]:	197.25
CAS:	86199-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-5.59	kJ/mol	Joback Method
hf	-231.10	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.188		Crippen Method
mvol	141.120	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	690.63	K	Joback Method
tc	977.61	K	Joback Method
tf	568.67	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.37	J/molxK	690.63	Joback Method
cpg	391.39	J/molxK	738.46	Joback Method
cpg	406.95	J/molxK	786.29	Joback Method
cpg	421.00	J/molxK	834.12	Joback Method
cpg	433.48	J/molxK	881.95	Joback Method
cpg	444.31	J/molxK	929.78	Joback Method
cpg	453.45	J/molxK	977.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86199395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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