

THIAZOLIDINE-2,4-DIONE

Inchi:	InChI=1S/C3H3NO2S/c5-2-1-7-3(6)4-2/h1H2,(H,4,5,6)
InchiKey:	ZOBPZXTWZATXDG-UHFFFAOYSA-N
Formula:	C3H3NO2S
SMILES:	O=C1CSC(=O)N1
Mol. weight [g/mol]:	117.13

Physical Properties

Property code	Value	Unit	Source
hfus	8.66	kJ/mol	Joback Method
logp	-0.031		Crippen Method
mcvol	71.740	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.24	J/mol×K	520.01	Joback Method
cpg	146.19	J/mol×K	565.42	Joback Method
cpg	154.90	J/mol×K	610.84	Joback Method
cpg	163.28	J/mol×K	656.25	Joback Method
cpg	171.22	J/mol×K	701.67	Joback Method
cpg	178.66	J/mol×K	747.08	Joback Method
cpg	185.49	J/mol×K	792.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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?Str2File=C2295310

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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