1-OXA-4-THIO-CYCLOHEXAN-2,6-DIONE

Other names: 1,4-Oxathiane-2,6-dione
1-Oxa-4-thia-cyclohexan-2,6-dione
Inchi: InChI=1S/C4H4O3S/c5-3-1-8-2-4(6)7-3/h1-2H2
InchiKey: RIIUAPMWDSRBSH-UHFFFAOYSA-N
Formula: C4H4O3S
SMILES: O=C1CSCC(=O)O1
Mol. weight [g/mol]: 132.14

Physical Properties

Property code	Value	Unit	Source
hf	-479.73	kJ/mol	Cheméo Relay (1.0)
hfus	7.54	kJ/mol	Joback Method
ie	9.83	eV	Cheméo Relay (1.0)
logp	-0.197		Crippen Method
mcvol	81.720	ml/mol	McGowan Method
tb	546.11	K	Cheméo Relay (1.0)
tf	442.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.85	J/mol×K	525.56	Joback Method
cpg	179.52	J/mol×K	570.37	Joback Method
cpg	189.77	J/mol×K	615.18	Joback Method
cpg	199.50	J/mol×K	659.99	Joback Method
cpg	208.64	J/mol×K	704.80	Joback Method
cpg	217.11	J/mol×K	749.60	Joback Method
cpg	224.82	J/mol×K	794.41	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3261878&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point