1,3-dimethylbicyclo[3.3.0]-2,8-dioxa-4-thiaoctane

Inchi: InChI=1S/C7H12O2S/c1-5-9-7(2)6(10-5)3-4-8-7/h5-6H,3-4H2,1-2H3
InchiKey: ZBNZQMIOTWVDDI-UHFFFAOYSA-N
Formula: C7H12O2S
SMILES: CC1OC2(C)OCCC2S1
Mol. weight [g/mol]: 160.23

Physical Properties

Property code	Value	Unit	Source
gf	-40.22	kJ/mol	Joback Method
hf	-278.37	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.601		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
ripol	1562.00		NIST Webbook
tb	478.88	K	Joback Method
tc	715.60	K	Joback Method
tf	353.74	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.87	J/mol×K	478.88	Joback Method
cpg	283.97	J/mol×K	518.33	Joback Method
cpg	298.71	J/mol×K	557.79	Joback Method
cpg	312.25	J/mol×K	597.24	Joback Method
cpg	324.78	J/mol×K	636.70	Joback Method
cpg	336.47	J/mol×K	676.15	Joback Method
cpg	347.48	J/mol×K	715.60	Joback Method

Sources

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=R169130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume