1,3-Propanediol, cyclic sulphate

Other names: 1,3-Propanediol, cyclic sulfate
1,3-Propylene sulfate
Trimethylene sulfate
1,3-Propanediol, cyclic sulphate
Inchi: InChI=1S/C3H6O4S/c4-8(5)6-2-1-3-7-8/h1-3H2
InchiKey: OQYOVYWFXHQYOP-UHFFFAOYSA-N
Formula: C3H6O4S
SMILES: O=S1(=O)OCCCO1
Mol. weight [g/mol]: 138.14

Physical Properties

Property code	Value	Unit	Source
hfus	21.15	kJ/mol	Joback Method
logp	-0.332		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
tf	334.20 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.99	J/mol×K	372.99	Joback Method
cpg	157.00	J/mol×K	405.75	Joback Method
cpg	166.53	J/mol×K	438.51	Joback Method
cpg	175.59	J/mol×K	471.27	Joback Method
cpg	184.20	J/mol×K	504.03	Joback Method
cpg	192.34	J/mol×K	536.79	Joback Method
cpg	200.03	J/mol×K	569.55	Joback Method

Sources

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?ID=C1073058&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point