1,4-Butanediol, cyclic sulphate

Inchi: InChI=1S/C4H8O4S/c5-9(6)7-3-1-2-4-8-9/h1-4H2
InchiKey: MGAFPXGQLWFEPK-UHFFFAOYSA-N
Formula: C4H8O4S
SMILES: O=S1(=O)OCCCCO1
Mol. weight [g/mol]: 152.17
CAS: 5732-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-631.18	kJ/mol	Joback Method
hf	-771.35	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.058		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	6663.89	kPa	Joback Method
tb	400.14	K	Joback Method
tc	603.69	K	Joback Method
tf	318.00 ± 3.00	K	NIST Webbook
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.02	J/mol×K	400.14	Joback Method
cpg	193.32	J/mol×K	434.06	Joback Method
cpg	205.05	J/mol×K	467.99	Joback Method
cpg	216.20	J/mol×K	501.91	Joback Method
cpg	226.77	J/mol×K	535.84	Joback Method
cpg	236.78	J/mol×K	569.76	Joback Method
cpg	246.21	J/mol×K	603.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5732445&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume