Busulfan

Inchi: InChI=1S/C6H14O6S2/c1-13(7,8)11-5-3-4-6-12-14(2,9)10/h3-6H2,1-2H3
InchiKey: COVZYZSDYWQREU-UHFFFAOYSA-N
Formula: C6H14O6S2
SMILES: CS(=O)(=O)OCCCCOS(C)(=O)=O
Mol. weight [g/mol]: 246.31

Physical Properties

Property code	Value	Unit	Source
gf	-1147.44	kJ/mol	Joback Method
hf	-1338.31	kJ/mol	Joback Method
hfus	36.43	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-2.27		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.281		Crippen Method
mcvol	163.320	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	477.08	K	Joback Method
tc	638.61	K	Joback Method
tf	278.96	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.86	J/mol×K	477.08	Joback Method
cpg	364.63	J/mol×K	504.00	Joback Method
cpg	376.09	J/mol×K	530.92	Joback Method
cpg	387.22	J/mol×K	557.85	Joback Method
cpg	398.00	J/mol×K	584.77	Joback Method
cpg	408.40	J/mol×K	611.69	Joback Method
cpg	418.41	J/mol×K	638.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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