

Thiamphenicol

Other names:	2,2-dichloro-N-[1,3-dihydroxy-1-(4-methylsulfonylphenyl)propan-2-yl]acetamide
Inchi:	InChI=1S/C12H15Cl2NO5S/c1-21(19,20)8-4-2-7(3-5-8)10(17)9(6-16)15-12(18)11(13)14/
InchiKey:	OTVAEFIXJLOWRX-UHFFFAOYSA-N
Formula:	C12H15Cl2NO5S
SMILES:	CS(=O)(=O)c1ccc(C(O)C(CO)NC(=O)C(Cl)Cl)cc1
Mol. weight [g/mol]:	356.23

Physical Properties

Property code	Value	Unit	Source
gf	-659.95	kJ/mol	Joback Method
hf	-930.19	kJ/mol	Joback Method
hfus	44.56	kJ/mol	Joback Method
hvap	118.02	kJ/mol	Joback Method
log10ws	-2.15		Estimated Solubility Method
log10ws	-2.15		Aqueous Solubility Prediction Method
logp	0.404		Crippen Method
mcvol	232.040	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	915.34	K	Joback Method
tc	1125.88	K	Joback Method
tf	438.30	K	Aqueous Solubility Prediction Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.63	J/molxK	915.34	Joback Method
cpg	658.25	J/molxK	950.43	Joback Method
cpg	664.97	J/molxK	985.52	Joback Method
cpg	670.82	J/molxK	1020.61	Joback Method
cpg	675.83	J/molxK	1055.70	Joback Method
cpg	680.03	J/molxK	1090.79	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

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