

Bromoxyleneol blue

Inchi:	InChI=1S/C23H20Br2O5S/c1-11-9-16(13(3)19(24)21(11)26)23(17-10-12(2)22(27)20(25)
InchiKey:	MRDOFVRMTNWMDA-UHFFFAOYSA-N
Formula:	C23H20Br2O5S
SMILES:	<chem>Cc1cc(C2(c3cc(C)c(O)c(Br)c3C)OS(=O)(=O)c3ccccc32)c(C)c(Br)c1O</chem>
Mol. weight [g/mol]:	568.27
CAS:	216771-60-7

Physical Properties

Property code	Value	Unit	Source
gf	-360.66	kJ/mol	Joback Method
hf	-684.63	kJ/mol	Joback Method
hfus	67.58	kJ/mol	Joback Method
hvap	138.05	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	5.867		Crippen Method
mcvol	333.490	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	1194.86	K	Joback Method
tc	1476.27	K	Joback Method
tf	1014.93	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.04	J/molxK	1194.86	Joback Method
cpg	1125.18	J/molxK	1241.76	Joback Method
cpg	1166.59	J/molxK	1288.66	Joback Method
cpg	1212.78	J/molxK	1335.57	Joback Method
cpg	1264.29	J/molxK	1382.47	Joback Method
cpg	1321.66	J/molxK	1429.37	Joback Method
cpg	1385.42	J/molxK	1476.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C216771607&Units=SI

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
mccvol:	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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