1,2-Benzenediol, 4-[2-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]amin

Other names: Protokylol

4-[2-[[2-(1,3-Benzodioxol-5-yl)-1-methylethyl]amino]-1-hydroxyethyl]-1,2-benzenediol hydrochloride

Cayfile

JB-251

Protokylol hydrochloride

Ventaire

Inchi: InChI=1S/C18H21NO5/c1-11(6-12-2-5-17-18(7-12)24-10-23-17)19-9-16(22)13-3-4-14(20

InchiKey: LUMAEVHDZXIGEP-UHFFFAOYSA-N

Formula: C18H21NO5

SMILES: CC(Cc1ccc2c(c1)OCO2)NCC(O)c1ccc(O)c(O)c1

Mol. weight [g/mol]: 331.36

CAS: 136-70-9

Physical Properties

Property code	Value	Unit	Source
gf	-159.09	kJ/mol	Joback Method
hf	-599.53	kJ/mol	Joback Method
hfus	56.41	kJ/mol	Joback Method
hvap	119.15	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.081		Crippen Method
mcvol	245.430	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	1042.58	K	Joback Method
tc	1286.90	K	Joback Method
tf	752.74	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.77	J/mol×K	1042.58	Joback Method
cpg	850.90	J/mol×K	1083.30	Joback Method
cpg	867.74	J/mol×K	1124.02	Joback Method

cpg	885.57	J/mol×K	1164.74	Joback Method
cpg	904.60	J/mol×K	1205.46	Joback Method
cpg	925.09	J/mol×K	1246.18	Joback Method
cpg	947.29	J/mol×K	1286.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136709&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