

Terbutaline

Inchi: InChI=1S/C12H19NO3/c1-12(2,3)13-7-11(16)8-4-9(14)6-10(15)5-8/h4-6,11,13-16H,7H2,
InchiKey: XWTYSIMOBUGWOL-UHFFFAOYSA-N
Formula: C12H19NO3
SMILES: CC(C)(C)NCC(O)c1cc(O)cc(O)c1
Mol. weight [g/mol]: 225.29
CAS: 23031-25-6

Physical Properties

Property code	Value	Unit	Source
hfus	30.69	kJ/mol	Joback Method
log10ws	-1.05		Cheméo Relay (1.0)
logp	1.519		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
tf	392.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-8.18390e+01
Coeff. B	1.61606e+00
Coeff. C	-1.42692e-03
Coeff. D	5.15000e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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