

Metaproterenol

Inchi:	InChI=1S/C11H17NO3/c1-7(2)12-6-11(15)8-3-9(13)5-10(14)4-8/h3-5,7,11-15H,6H2,1-2H
InchiKey:	LMOINURANNBYCM-UHFFFAOYSA-N
Formula:	C11H17NO3
SMILES:	CC(C)NCC(O)c1cc(O)cc(O)c1
Mol. weight [g/mol]:	211.26
CAS:	586-06-1

Physical Properties

Property code	Value	Unit	Source
hf	-493.06	kJ/mol	Cheméo Relay (1.0)
hfus	31.99	kJ/mol	Joback Method
log10ws	-0.58		Cheméo Relay (1.0)
logp	1.129		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
tf	373.15	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	-5.81390e+01
Coeff. B	1.40114e+00
Coeff. C	-1.20392e-03
Coeff. D	4.30700e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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
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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
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

Latest version available from:

<https://www.chemeo.com/cid/112-228-4/Metaproterenol.pdf>

Generated by Cheméo on 2026-10-28 01:22:58.14447434 +0000 UTC m=+15621.207375773.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.