

Emodin

Inchi:	InChI=1S/C15H10O5/c1-6-2-8-12(10(17)3-6)15(20)13-9(14(8)19)4-7(16)5-11(13)18/h2-5
InchiKey:	RHMXXJGYXNZAPX-UHFFFAOYSA-N
Formula:	C15H10O5
SMILES:	Cc1cc(O)c2c(c1)C(=O)c1cc(O)cc(O)c1C2=O
Mol. weight [g/mol]:	270.24
CAS:	518-82-1

Physical Properties

Property code	Value	Unit	Source
hfus	37.05	kJ/mol	Joback Method
logp	1.887		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
tf	530.15	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	-4.06200e+01
Coeff. B	1.40672e+00
Coeff. C	-1.25656e-03
Coeff. D	4.74300e-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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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