Chrysophanol

Inchi: InChI=1S/C15H10O4/c1-7-5-9-13(11(17)6-7)15(19)12-8(14(9)18)3-2-4-10(12)16/h2-6,16
InchiKey: LQGUBLBATBMXHT-UHFFFAOYSA-N
Formula: C15H10O4
SMILES: Cc1cc(O)c2c(c1)C(=O)c1cccc(O)c1C2=O
Mol. weight [g/mol]: 254.24
CAS: 481-74-3

Physical Properties

Property code	Value	Unit	Source
hf	-472.96	kJ/mol	Cheméo Relay (1.0)
hfus	31.27	kJ/mol	Joback Method
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-4.48		Cheméo Relay (1.0)
logp	2.182		Crippen Method
mcvol	178.710	ml/mol	McGowan Method
tf	469.15	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	-3.17000e+01
Coeff. B	1.25212e+00
Coeff. C	-1.00020e-03
Coeff. D	3.41200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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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