Fluorescein

Inchi: InChI=1S/C20H12O5/c21-11-5-7-15-17(9-11)24-18-10-12(22)6-8-16(18)20(15)14-4-2-1-3
InchiKey: GNBHRKFJIUUOQI-UHFFFAOYSA-N
Formula: C20H12O5
SMILES: O=C1OC2(c3ccc(O)cc3Oc3cc(O)ccc32)c2ccccc21
Mol. weight [g/mol]: 332.31
CAS: 2321-07-5

Physical Properties

Property code	Value	Unit	Source
hfus	49.73	kJ/mol	Joback Method
log10ws	-5.06		Cheméo Relay (1.0)
logp	3.666		Crippen Method
mcvol	224.710	ml/mol	McGowan Method
tf	590.65	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	-1.85150e+02
Coeff. B	2.39860e+00
Coeff. C	-2.57490e-03
Coeff. D	1.07340e-06
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
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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