

# 4',5'-Diiodofluorescein

<b>Inchi:</b>	InChI=1S/C20H12I2O5/c21-16-13(23)7-5-11-15(9-3-1-2-4-10(9)20(25)26)12-6-8-14(24)1
<b>InchiKey:</b>	SGBGBWVDANLPDL-UHFFFAOYSA-N
<b>Formula:</b>	C20H12I2O5
<b>SMILES:</b>	O=C1C=CC2=C(c3ccccc3C(=O)O)C3C=CC(O)=C(I)C3OC2=C1I
<b>Mol. weight [g/mol]:</b>	586.12

## Physical Properties

Property code	Value	Unit	Source
gf	-53.25	kJ/mol	Joback Method
hf	-336.05	kJ/mol	Joback Method
hfus	53.89	kJ/mol	Joback Method
hvap	137.00	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	4.713		Crippen Method
mcvol	287.210	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
tb	1279.86	K	Joback Method
tc	1570.00	K	Joback Method
tf	855.96	K	Joback Method
vc	1.058	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.11	J/mol×K	1279.86	Joback Method
cpg	822.91	J/mol×K	1328.22	Joback Method
cpg	830.62	J/mol×K	1376.57	Joback Method
cpg	838.40	J/mol×K	1424.93	Joback Method
cpg	846.42	J/mol×K	1473.29	Joback Method
cpg	854.84	J/mol×K	1521.64	Joback Method
cpg	863.82	J/mol×K	1570.00	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002856&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002856&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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