

6H,12H-Dibenzo[b,f][1,5]dioxocin-6,12-dione

Other names:	Benzoic acid, 2-hydroxy-, bimol. cyclic ester Disalicylide Salicylic acid, bimol. cyclic ester 6H,12H-Dibenzo[b,f][1,5]dioxocine-6,12-dione
Inchi:	InChI=1S/C14H8O4/c15-13-9-5-1-3-7-11(9)17-14(16)10-6-2-4-8-12(10)18-13/h1-8H
InchiKey:	MLSVGAXOQBMEGH-UHFFFAOYSA-N
Formula:	C14H8O4
SMILES:	O=C1Oc2ccccc2C(=O)Oc2ccccc21
Mol. weight [g/mol]:	240.21
CAS:	486-58-8

Physical Properties

Property code	Value	Unit	Source
gf	-88.50	kJ/mol	Joback Method
hf	-334.59	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.438		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	788.26	K	Joback Method
tc	1070.21	K	Joback Method
tf	533.66	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.03	J/molxK	788.26	Joback Method
cpg	475.53	J/molxK	835.25	Joback Method
cpg	487.48	J/molxK	882.24	Joback Method

cpg	497.88	J/mol×K	929.23	Joback Method
cpg	506.74	J/mol×K	976.23	Joback Method
cpg	514.05	J/mol×K	1023.22	Joback Method
cpg	519.84	J/mol×K	1070.21	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C486588&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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