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

Physical Properties

Property code	Value	Unit	Source
hf	-426.68	kJ/mol	Cheméo Relay (1.0)
hfus	29.26	kJ/mol	Joback Method
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-4.60		Cheméo Relay (1.0)
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	646.64	K	Cheméo Relay (1.0)
tc	949.23	K	Cheméo Relay (1.0)
tf	461.64	K	Cheméo Relay (1.0)
vc	0.611	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C486588&Units=SI

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

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
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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