RESORCINOL BENZOATE

Other names:	Resorcinol dibenzoate
	1,3-Dibenzoyloxybenzene
	1,3-Benzenediol, dibenzoate
	1,3-Bis(benzoyloxy)benzene
	3-(Benzoyloxy)phenyl benzoate
	m-phenylene dibenzoate
	Dibenzoyl resorcinol
Inchi:	InChI=1S/C20H14O4/c21-19(15-8-3-1-4-9-15)23-17-12-7-13-18(14-17)24-20(22)16-10-5
InchiKey:	SUQGLJRNDJRARS-UHFFFAOYSA-N
Formula:	C20H14O4
SMILES:	O=C(Oc1cccc(OC(=O)c2ccccc2)c1)c1ccccc1
Mol. weight [g/mol]:	318.33

Physical Properties

Property code	Value	Unit	Source
af	0.8112		Cheméo Relay (1.0)
gf	-22.72	kJ/mol	Joback Method
hf	-351.49	kJ/mol	Cheméo Relay (1.0)
hfus	34.86	kJ/mol	Joback Method
hvap	113.97	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	Cheméo Relay (1.0)
log10ws	-5.33		Cheméo Relay (1.0)
logp	4.125		Crippen Method
mcvol	236.260	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	677.16	K	Cheméo Relay (1.0)
tc	991.03	K	Cheméo Relay (1.0)
tf	375.06	K	Cheméo Relay (1.0)
vc	0.871	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.98	J/mol×K	1152.17	Joback Method

cpg	720.18	J/mol×K	1066.32	Joback Method
cpg	680.56	J/mol×K	894.60	Joback Method
cpg	692.64	J/mol×K	937.53	Joback Method
cpg	703.23	J/mol×K	980.46	Joback Method
cpg	712.38	J/mol×K	1023.39	Joback Method
cpg	726.69	J/mol×K	1109.24	Joback Method
dvisc	0.0004589	Pa×s	551.26	Joback Method
dvisc	0.0002761	Pa×s	608.48	Joback Method
dvisc	0.0001812	Pa×s	665.71	Joback Method
dvisc	0.0001272	Pa×s	722.93	Joback Method
dvisc	0.0000940	Pa×s	780.15	Joback Method
dvisc	0.0000724	Pa×s	837.38	Joback Method
dvisc	0.0000577	Pa×s	894.60	Joback Method
hsubt	165.80	kJ/mol	361.00	NIST Webbook
hvapt	76.00	kJ/mol	446.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94019&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

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume