

o-Dibenzoyl benzene

Other names:	ortho-Dibenzoylbenzene 1,2-Dibenzoylbenzene 2-Benzoylbenzophenone Methanone, 1,2-phenylenebis[phenyl- Benzene, o-dibenzoyl- o-Benzoylbenzophenone
Inchi:	InChI=1S/C20H14O2/c21-19(15-9-3-1-4-10-15)17-13-7-8-14-18(17)20(22)16-11-5-2-6-12
InchiKey:	OJLABXSUFRIXFL-UHFFFAOYSA-N
Formula:	C20H14O2
SMILES:	O=C(c1ccccc1)c1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]:	286.33

Physical Properties

Property code	Value	Unit	Source
af	0.6671		Cheméo Relay (1.0)
gf	187.28	kJ/mol	Joback Method
hf	17.51	kJ/mol	Cheméo Relay (1.0)
hfus	32.49	kJ/mol	Joback Method
hvap	120.09	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
log10ws	-5.22		Cheméo Relay (1.0)
logp	4.149		Crippen Method
mcvol	224.520	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
tb	669.11	K	Cheméo Relay (1.0)
tc	995.34	K	Cheméo Relay (1.0)
tf	389.20	K	Cheméo Relay (1.0)
vc	0.822	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.61	J/mol×K	849.76	Joback Method
cpg	643.27	J/mol×K	894.04	Joback Method

cpg	655.54	J/mol×K	938.32	Joback Method
cpg	666.56	J/mol×K	982.60	Joback Method
cpg	676.45	J/mol×K	1026.88	Joback Method
cpg	685.36	J/mol×K	1071.16	Joback Method
cpg	693.41	J/mol×K	1115.44	Joback Method
dvisc	0.0008865	Pa×s	506.80	Joback Method
dvisc	0.0005130	Pa×s	563.96	Joback Method
dvisc	0.0003283	Pa×s	621.12	Joback Method
dvisc	0.0002265	Pa×s	678.28	Joback Method
dvisc	0.0001656	Pa×s	735.44	Joback Method
dvisc	0.0001266	Pa×s	792.60	Joback Method
dvisc	0.0001004	Pa×s	849.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1159860&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

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
hvap:	Enthalpy of vaporization 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
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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