

o-Dibenzoylbenzene

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]:	286.32
CAS:	1159-86-0

Physical Properties

Property code	Value	Unit	Source
gf	187.28	kJ/mol	Joback Method
hf	16.83	kJ/mol	Joback Method
hfus	32.49	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.149		Crippen Method
mcvol	224.520	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
tb	849.76	K	Joback Method
tc	1115.44	K	Joback Method
tf	506.80	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.61	J/molxK	849.76	Joback Method
cpg	643.27	J/molxK	894.04	Joback Method
cpg	655.54	J/molxK	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	Paxs	506.80	Joback Method
dvisc	0.0005130	Paxs	563.96	Joback Method
dvisc	0.0003283	Paxs	621.12	Joback Method
dvisc	0.0002265	Paxs	678.28	Joback Method
dvisc	0.0001656	Paxs	735.44	Joback Method
dvisc	0.0001266	Paxs	792.60	Joback Method
dvisc	0.0001004	Paxs	849.76	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=C1159860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
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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