1,3-Dibenzoylbenzene

Other names: m-Dibenzoylbenzene
Methanone, 1,3-phenylenebis[phenyl-
Inchi: InChI=1S/C20H14O2/c21-19(15-8-3-1-4-9-15)17-12-7-13-18(14-17)20(22)16-10-5-2-6-11
InchiKey: MJQHDSIEDGPFAM-UHFFFAOYSA-N
Formula: C20H14O2
SMILES: O=C(c1ccccc1)c1cccc(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 286.32
CAS: 3770-82-9

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/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3770829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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