

2,4-Dibenzoyl resorcinol

Inchi:	InChI=1S/C20H14O4/c21-16-12-11-15(18(22)13-7-3-1-4-8-13)20(24)17(16)19(23)14-9-5
InchiKey:	KOKLAVMEUFYRKV-UHFFFAOYSA-N
Formula:	C20H14O4
SMILES:	O=C(c1ccccc1)c1ccc(O)c(C(=O)c2ccccc2)c1O
Mol. weight [g/mol]:	318.32
CAS:	82-64-4

Physical Properties

Property code	Value	Unit	Source
gf	-121.96	kJ/mol	Joback Method
hf	-337.79	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	107.12	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.560		Crippen Method
mcvol	236.260	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	1011.00	K	Joback Method
tc	1285.56	K	Joback Method
tf	730.24	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.80	J/mol×K	1011.00	Joback Method
cpg	733.04	J/mol×K	1056.76	Joback Method
cpg	747.72	J/mol×K	1102.52	Joback Method
cpg	763.12	J/mol×K	1148.28	Joback Method
cpg	779.57	J/mol×K	1194.04	Joback Method
cpg	797.35	J/mol×K	1239.80	Joback Method
cpg	816.78	J/mol×K	1285.56	Joback Method
dvisc	0.0000021	Pa×s	730.24	Joback Method
dvisc	0.0000011	Pa×s	777.03	Joback Method

dvisc	0.0000006	Pa×s	823.83	Joback Method
dvisc	0.0000004	Pa×s	870.62	Joback Method
dvisc	0.0000002	Pa×s	917.41	Joback Method
dvisc	0.0000002	Pa×s	964.21	Joback Method
dvisc	0.0000001	Pa×s	1011.00	Joback Method

Sources

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=C82644&Units=SI
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
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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