1,2-Benzenedicarboxylic acid, diphenyl ester

Other names: Phthalic acid, diphenyl ester
Diphenyl phthalate
Phenyl phthalate
Inchi: InChI=1S/C20H14O4/c21-19(23-15-9-3-1-4-10-15)17-13-7-8-14-18(17)20(22)24-16-11-5
InchiKey: DWNAQMUDCDVSLT-UHFFFAOYSA-N
Formula: C20H14O4
SMILES: O=C(Oc1ccccc1)c1ccccc1C(=O)Oc1ccccc1
Mol. weight [g/mol]: 318.32
CAS: 84-62-8

Physical Properties

Property code	Value	Unit	Source
chs	-9381.80 ± 9.20	kJ/mol	NIST Webbook
gf	-22.72	kJ/mol	Joback Method
hf	-247.61	kJ/mol	Joback Method
hfs	-489.20 ± 9.20	kJ/mol	NIST Webbook
hfus	34.86	kJ/mol	Joback Method
hvap	85.92	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.125		Crippen Method
mcvol	236.260	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2500.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	894.60	K	Joback Method
tc	1152.17	K	Joback Method
tf	551.26	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	680.56	J/mol×K	894.60	Joback Method
cpg	726.69	J/mol×K	1109.24	Joback Method
cpg	720.18	J/mol×K	1066.32	Joback Method
cpg	712.38	J/mol×K	1023.39	Joback Method
cpg	703.23	J/mol×K	980.46	Joback Method
cpg	692.64	J/mol×K	937.53	Joback Method
cpg	731.98	J/mol×K	1152.17	Joback Method
dvisc	0.0000577	Pa×s	894.60	Joback Method
dvisc	0.0000724	Pa×s	837.38	Joback Method
dvisc	0.0000940	Pa×s	780.15	Joback Method
dvisc	0.0001272	Pa×s	722.93	Joback Method
dvisc	0.0001812	Pa×s	665.71	Joback Method
dvisc	0.0002761	Pa×s	608.48	Joback Method
dvisc	0.0004589	Pa×s	551.26	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=C84628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
rinpol:	Non-polar retention indices

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