DIPHENYL ISOPHTHALATE

Other names: 1,3-Benzenedicarboxylic acid, diphenyl ester
Diphenyl m-phthalate
Isophthalic acid, diphenyl ester
Inchi: InChI=1S/C20H14O4/c21-19(23-17-10-3-1-4-11-17)15-8-7-9-16(14-15)20(22)24-18-12-5
InchiKey: FHESUNXRPBHDQM-UHFFFAOYSA-N
Formula: C20H14O4
SMILES: O=C(Oc1ccccc1)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 318.33

Physical Properties

Property code	Value	Unit	Source
af	0.8094		Cheméo Relay (1.0)
gf	-22.72	kJ/mol	Joback Method
hf	-354.65	kJ/mol	Cheméo Relay (1.0)
hfs	-476.10	kJ/mol	NIST Webbook
hfus	34.86	kJ/mol	Joback Method
hvap	105.77	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-5.26		Cheméo Relay (1.0)
logp	4.125		Crippen Method
mcvol	236.260	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	675.33	K	Cheméo Relay (1.0)
tc	991.34	K	Cheméo Relay (1.0)
tf	381.70	K	Cheméo Relay (1.0)
vc	0.869	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.56	J/mol×K	894.60	Joback Method
cpg	692.64	J/mol×K	937.53	Joback Method
cpg	703.23	J/mol×K	980.46	Joback Method
cpg	712.38	J/mol×K	1023.39	Joback Method

cpg	720.18	J/mol×K	1066.32	Joback Method
cpg	726.69	J/mol×K	1109.24	Joback Method
cpg	731.98	J/mol×K	1152.17	Joback Method
dvisc	0.0004589	Pa×s	551.26	Joback Method
dvisc	0.0002761	Pa×s	608.48	Joback Method
dvisc	0.0001812	Pa×s	665.71	Joback Method
dvisc	0.0001272	Pa×s	722.93	Joback Method
dvisc	0.0000940	Pa×s	780.15	Joback Method
dvisc	0.0000724	Pa×s	837.38	Joback Method
dvisc	0.0000577	Pa×s	894.60	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C744456&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfs: Solid phase 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