1,2-Benzenedicarboxylic acid, bis(1-methylethyl) ester

Other names: Phthalic acid, diisopropyl ester
Diisopropyl phthalate
Inchi: InChI=1S/C14H18O4/c1-9(2)17-13(15)11-7-5-6-8-12(11)14(16)18-10(3)4/h5-10H,1-4H3
InchiKey: QWDBCIAVABMJPP-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CC(C)OC(=O)c1ccccc1C(=O)OC(C)C
Mol. weight [g/mol]: 250.29
CAS: 605-45-8

Physical Properties

Property code	Value	Unit	Source
gf	-302.94	kJ/mol	Joback Method
hf	-607.39	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.817		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	295.40		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	295.40		NIST Webbook
rinpol	1641.00		NIST Webbook
tb	703.08	K	Joback Method
tc	916.20	K	Joback Method
tf	400.80	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.05	J/mol×K	916.20	Joback Method

cpg	605.95	J/mol×K	880.68	Joback Method
cpg	594.90	J/mol×K	845.16	Joback Method
cpg	582.89	J/mol×K	809.64	Joback Method
cpg	569.92	J/mol×K	774.12	Joback Method
cpg	555.97	J/mol×K	738.60	Joback Method
cpg	541.05	J/mol×K	703.08	Joback Method
dvisc	0.0013715	Pa×s	400.80	Joback Method
dvisc	0.0001019	Pa×s	703.08	Joback Method
dvisc	0.0001330	Pa×s	652.70	Joback Method
dvisc	0.0001815	Pa×s	602.32	Joback Method
dvisc	0.0002620	Pa×s	551.94	Joback Method
dvisc	0.0004071	Pa×s	501.56	Joback Method
dvisc	0.0006983	Pa×s	451.18	Joback Method
hvapt	74.80	kJ/mol	430.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C605458&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hvapt: Enthalpy of vaporization at a given temperature
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