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

Other names: 1,2-Benzenedicarboxylic acid, 1,2-bis(2-methylpropyl) ester
1,2-Benzenedicarboxylic acid, di(2-methylpropyl) ester
Bis(2-methylpropyl) phthalate
DIBP
DIISOBUTYL ESTER
Diisobutyl phthalate
Diisobutylester kyseliny ftalove
Hexaplas M/1B
ISOBUTYL PHTHALATE
Isobutyl-o-phthalate
Kodaflex DIBP
NSC 15316
PHTHALIC ACID
Palatinol IC
Phthalic acid, diisobutyl ester
bis(2-methylpropyl) benzene-1,2-dicarboxylate
di-2-methylpropyl phthalate

Inchi: InChI=1S/C16H22O4/c1-11(2)9-19-15(17)13-7-5-6-8-14(13)16(18)20-10-12(3)4/h5-8,11-

InchiKey: MGWAVDBGNNKXQV-UHFFFAOYSA-N

Formula: C16H22O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 278.34

CAS: 84-69-5

Physical Properties

Property code	Value	Unit	Source
gf	-286.10	kJ/mol	Joback Method
hf	-648.67	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-4.68		Aqueous Solubility Prediction Method
logp	3.312		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1870.90		NIST Webbook

rinpol	1871.80	NIST Webbook
rinpol	316.60	NIST Webbook
rinpol	1871.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1826.00	NIST Webbook
rinpol	1847.00	NIST Webbook
rinpol	316.60	NIST Webbook
rinpol	1863.00	NIST Webbook
rinpol	1871.80	NIST Webbook
rinpol	1868.00	NIST Webbook
rinpol	1873.00	NIST Webbook
rinpol	1867.50	NIST Webbook
rinpol	1867.80	NIST Webbook
rinpol	1870.90	NIST Webbook
rinpol	1874.30	NIST Webbook
rinpol	1876.00	NIST Webbook
rinpol	1819.00	NIST Webbook
rinpol	1862.00	NIST Webbook
rinpol	1871.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1916.00	NIST Webbook
rinpol	1869.00	NIST Webbook
rinpol	1853.00	NIST Webbook
rinpol	1877.00	NIST Webbook
rinpol	1826.00	NIST Webbook
rinpol	1819.00	NIST Webbook
rinpol	1871.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1908.00	NIST Webbook
rinpol	1869.00	NIST Webbook
rinpol	1897.00	NIST Webbook
rinpol	1868.00	NIST Webbook
rinpol	1875.00	NIST Webbook
rinpol	1871.00	NIST Webbook
rinpol	1873.00	NIST Webbook
rinpol	1877.00	NIST Webbook
rinpol	1866.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1847.00	NIST Webbook
rinpol	1863.00	NIST Webbook
rinpol	1869.00	NIST Webbook
rinpol	1868.00	NIST Webbook
rinpol	1863.00	NIST Webbook

ripol	2536.00		NIST Webbook
ripol	2536.00		NIST Webbook
ripol	2548.00		NIST Webbook
ripol	2548.00		NIST Webbook
ripol	2526.00		NIST Webbook
ripol	2592.00		NIST Webbook
tb	593.00 ± 4.00	K	NIST Webbook
tc	956.66	K	Joback Method
tf	423.34	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.54	J/mol×K	748.84	Joback Method
cpg	717.14	J/mol×K	922.02	Joback Method
cpg	705.67	J/mol×K	887.39	Joback Method
cpg	693.19	J/mol×K	852.75	Joback Method
cpg	679.68	J/mol×K	818.11	Joback Method
cpg	665.13	J/mol×K	783.48	Joback Method
cpg	727.62	J/mol×K	956.66	Joback Method
dvisc	0.0000793	Pa×s	748.84	Joback Method
dvisc	0.0001042	Pa×s	694.59	Joback Method
dvisc	0.0001432	Pa×s	640.34	Joback Method
dvisc	0.0002089	Pa×s	586.09	Joback Method
dvisc	0.0003291	Pa×s	531.84	Joback Method
dvisc	0.0005749	Pa×s	477.59	Joback Method
dvisc	0.0011585	Pa×s	423.34	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1158.mol

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C84695&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume