1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester

Other names: Phthalic acid, butyl isobutyl ester
1-Butyl 2-isobutyl phthalate
2-Methylpropyl butyl phthalate
Butyl isobutyl phthalate

Inchi: InChI=1S/C16H22O4/c1-4-5-10-19-15(17)13-8-6-7-9-14(13)16(18)20-11-12(2)3/h6-9,12H

InchiKey: UVIVWIFUPKGWGF-UHFFFAOYSA-N

Formula: C16H22O4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 278.34

CAS: 17851-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-283.66	kJ/mol	Joback Method
hf	-643.39	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.456		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	749.28	K	Joback Method
tc	954.00	K	Joback Method
tf	438.34	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.00	J/mol×K	749.28	Joback Method
cpg	715.80	J/mol×K	919.88	Joback Method
cpg	704.40	J/mol×K	885.76	Joback Method
cpg	692.04	J/mol×K	851.64	Joback Method
cpg	678.69	J/mol×K	817.52	Joback Method
cpg	664.35	J/mol×K	783.40	Joback Method
cpg	726.23	J/mol×K	954.00	Joback Method
dvisc	0.0000861	Pa×s	749.28	Joback Method
dvisc	0.0001111	Pa×s	697.46	Joback Method
dvisc	0.0001494	Pa×s	645.63	Joback Method
dvisc	0.0002115	Pa×s	593.81	Joback Method
dvisc	0.0003201	Pa×s	541.99	Joback Method
dvisc	0.0005289	Pa×s	490.16	Joback Method
dvisc	0.0009839	Pa×s	438.34	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=C17851535&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume