1,2-Benzenedicarboxylic acid, monobutyl ester

Other names: Phthalic acid, monobutyl ester
Butyl hydrogen phthalate
Monobutyl phthalate
Mono-n-butyl phthalate
MBP

Inchi: InChI=1S/C12H14O4/c1-2-3-8-16-12(15)10-7-5-4-6-9(10)11(13)14/h4-7H,2-3,8H2,1H3,(H

InchiKey: YZBOVSFWWNVKRJ-UHFFFAOYSA-N

Formula: C12H14O4

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

Mol. weight [g/mol]: 222.24

CAS: 131-70-4

Physical Properties

Property code	Value	Unit	Source
gf	-346.72	kJ/mol	Joback Method
hf	-575.56	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.342		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook
tb	727.96	K	Joback Method
tc	929.50	K	Joback Method
tf	446.85	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.63	J/mol×K	727.96	Joback Method
cpg	510.63	J/mol×K	895.91	Joback Method

cpg	502.40	J/mol×K	862.32	Joback Method
cpg	493.50	J/mol×K	828.73	Joback Method
cpg	483.92	J/mol×K	795.14	Joback Method
cpg	473.63	J/mol×K	761.55	Joback Method
cpg	518.21	J/mol×K	929.50	Joback Method
dvisc	0.0000419	Pa×s	727.96	Joback Method
dvisc	0.0000597	Pa×s	681.11	Joback Method
dvisc	0.0000898	Pa×s	634.26	Joback Method
dvisc	0.0001440	Pa×s	587.40	Joback Method
dvisc	0.0002506	Pa×s	540.55	Joback Method
dvisc	0.0004846	Pa×s	493.70	Joback Method
dvisc	0.0010761	Pa×s	446.85	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=C131704&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