1,2-Benzenedicarboxylic acid, butyl methyl ester

Other names: Phthalic acid, butyl methyl ester
Butyl methyl phthalate
Methyl butyl phthalate

Inchi: InChI=1S/C13H16O4/c1-3-4-9-17-13(15)11-8-6-5-7-10(11)12(14)16-2/h5-8H,3-4,9H2,1-2

InchiKey: XXFSYINDUHLBIL-UHFFFAOYSA-N

Formula: C13H16O4

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

Mol. weight [g/mol]: 236.26

CAS: 34006-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-306.48	kJ/mol	Joback Method
hf	-576.19	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.430		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
tb	681.08	K	Joback Method
tc	889.77	K	Joback Method
tf	419.53	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.57	J/mol×K	681.08	Joback Method
cpg	548.61	J/mol×K	854.99	Joback Method
cpg	538.09	J/mol×K	820.20	Joback Method
cpg	526.74	J/mol×K	785.42	Joback Method

cpg	514.53	J/mol×K	750.64	Joback Method
cpg	501.48	J/mol×K	715.86	Joback Method
cpg	558.29	J/mol×K	889.77	Joback Method
dvisc	0.0001337	Pa×s	681.08	Joback Method
dvisc	0.0001677	Pa×s	637.49	Joback Method
dvisc	0.0002173	Pa×s	593.90	Joback Method
dvisc	0.0002935	Pa×s	550.30	Joback Method
dvisc	0.0004175	Pa×s	506.71	Joback Method
dvisc	0.0006345	Pa×s	463.12	Joback Method
dvisc	0.0010519	Pa×s	419.53	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34006763&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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