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

Other names: Butyl 2-ethylhexyl phthalate
Butyl, 2-ethylhexylphthalated
O2-butyl O1-(2-ethylhexyl) benzene-1,2-dicarboxylate
Phthalic acid, butyl 2-ethylhexyl ester

Inchi: InChI=1S/C20H30O4/c1-4-7-11-16(6-3)15-24-20(22)18-13-10-9-12-17(18)19(21)23-14-8

InchiKey: AVOLBYOSCILFLL-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 334.45

CAS: 85-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-249.98	kJ/mol	Joback Method
hf	-725.95	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	80.98	kJ/mol	Joback Method
log10ws	-7.22		Aqueous Solubility Prediction Method
logp	5.017		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
tb	840.80	K	Joback Method
tc	1042.55	K	Joback Method
tf	483.42	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.24	J/mol×K	840.80	Joback Method
cpg	894.49	J/mol×K	874.43	Joback Method
cpg	909.59	J/mol×K	908.05	Joback Method
cpg	923.56	J/mol×K	941.68	Joback Method

cpg	936.41	J/mol×K	975.30	Joback Method
cpg	948.18	J/mol×K	1008.93	Joback Method
cpg	958.87	J/mol×K	1042.55	Joback Method
dvisc	0.0006723	Pa×s	483.42	Joback Method
dvisc	0.0003442	Pa×s	542.98	Joback Method
dvisc	0.0002012	Pa×s	602.55	Joback Method
dvisc	0.0001295	Pa×s	662.11	Joback Method
dvisc	0.0000897	Pa×s	721.67	Joback Method
dvisc	0.0000656	Pa×s	781.24	Joback Method
dvisc	0.0000502	Pa×s	840.80	Joback Method

Sources

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

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=C85698&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume