1,2-Benzenedicarboxylic acid, butyl cyclohexyl ester

Other names: Phthalic acid, butyl cyclohexyl ester
Butyl cyclohexyl phthalate
Cyclohexyl butyl phthalate
Elastex 50B
1-Butyl 2-cyclohexyl phthalate

Inchi: InChI=1S/C18H24O4/c1-2-3-13-21-17(19)15-11-7-8-12-16(15)18(20)22-14-9-5-4-6-10-14

InchiKey: BHKLONWXRPJNAE-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OC1CCCCC1

Mol. weight [g/mol]: 304.38

CAS: 84-64-0

Physical Properties

Property code	Value	Unit	Source
gf	-239.93	kJ/mol	Joback Method
hf	-625.07	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.133		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
tb	815.03	K	Joback Method
tc	1038.33	K	Joback Method
tf	483.26	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.87	J/mol×K	815.03	Joback Method
cpg	772.90	J/mol×K	852.25	Joback Method
cpg	788.49	J/mol×K	889.46	Joback Method
cpg	802.66	J/mol×K	926.68	Joback Method

cpg	815.43	J/mol×K	963.90	Joback Method
cpg	826.83	J/mol×K	1001.11	Joback Method
cpg	836.90	J/mol×K	1038.33	Joback Method
dvisc	0.0008245	Pa×s	483.26	Joback Method
dvisc	0.0004502	Pa×s	538.55	Joback Method
dvisc	0.0002751	Pa×s	593.85	Joback Method
dvisc	0.0001828	Pa×s	649.14	Joback Method
dvisc	0.0001296	Pa×s	704.44	Joback Method
dvisc	0.0000965	Pa×s	759.73	Joback Method
dvisc	0.0000749	Pa×s	815.03	Joback Method
hvapt	94.30	kJ/mol	426.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C84640&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
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