1,2-Cyclohexanedicarboxylic acid, butyl cyclohexyl ester

Inchi: InChI=1S/C18H30O4/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: LZLBAKBZXZWMPZ-UHFFFAOYSA-N

Formula: C18H30O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-325.97	kJ/mol	Joback Method
hf	-816.15	kJ/mol	Joback Method
hfus	32.69	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.012		Crippen Method
mcvol	257.640	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
tb	798.25	K	Joback Method
tc	1015.58	K	Joback Method
tf	447.46	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.52	J/mol×K	798.25	Joback Method
cpg	866.22	J/mol×K	834.47	Joback Method
cpg	885.24	J/mol×K	870.69	Joback Method
cpg	902.61	J/mol×K	906.91	Joback Method
cpg	918.35	J/mol×K	943.13	Joback Method
cpg	932.48	J/mol×K	979.36	Joback Method
cpg	945.01	J/mol×K	1015.58	Joback Method
dvisc	0.0014280	Pa×s	447.46	Joback Method

dvisc	0.0007032	Pa×s	505.92	Joback Method
dvisc	0.0004011	Pa×s	564.39	Joback Method
dvisc	0.0002542	Pa×s	622.86	Joback Method
dvisc	0.0001742	Pa×s	681.32	Joback Method
dvisc	0.0001267	Pa×s	739.79	Joback Method
dvisc	0.0000966	Pa×s	798.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339760&Units=SI
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

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