1,2-Cyclohexanedicarboxylic acid, butyl pentyl ester

Inchi: InChI=1S/C17H30O4/c1-3-5-9-13-21-17(19)15-11-8-7-10-14(15)16(18)20-12-6-4-2/h14-1
InchiKey: MHLAFTPJAGNOOB-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCCCC
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-358.84	kJ/mol	Joback Method
hf	-849.83	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	71.87	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.870		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	755.82	K	Joback Method
tc	950.83	K	Joback Method
tf	428.81	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.64	J/mol×K	755.82	Joback Method
cpg	872.45	J/mol×K	918.33	Joback Method
cpg	858.22	J/mol×K	885.83	Joback Method
cpg	842.83	J/mol×K	853.33	Joback Method
cpg	826.28	J/mol×K	820.82	Joback Method
cpg	808.55	J/mol×K	788.32	Joback Method
cpg	885.53	J/mol×K	950.83	Joback Method
dvisc	0.0001055	Pa×s	755.82	Joback Method

dvisc	0.0001368	Pa×s	701.32	Joback Method
dvisc	0.0001852	Pa×s	646.82	Joback Method
dvisc	0.0002653	Pa×s	592.31	Joback Method
dvisc	0.0004086	Pa×s	537.81	Joback Method
dvisc	0.0006936	Pa×s	483.31	Joback Method
dvisc	0.0013472	Pa×s	428.81	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=U339466&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