1,2-Cyclohexanedicarboxylic acid, butyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C19H32O4/c1-3-4-13-22-18(20)15-10-6-7-11-16(15)19(21)23-17-12-8-5-9-14(1

InchiKey: PUUCICBQTSLTHS-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-325.26	kJ/mol	Joback Method
hf	-857.13	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	76.44	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.258		Crippen Method
mcvol	271.730	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	816.46	K	Joback Method
tc	1031.59	K	Joback Method
tf	454.49	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.91	J/mol×K	816.46	Joback Method
cpg	996.50	J/mol×K	995.73	Joback Method
cpg	982.39	J/mol×K	959.88	Joback Method
cpg	966.59	J/mol×K	924.02	Joback Method
cpg	949.08	J/mol×K	888.17	Joback Method
cpg	929.86	J/mol×K	852.31	Joback Method
cpg	1008.93	J/mol×K	1031.59	Joback Method
dvisc	0.0001078	Pa×s	816.46	Joback Method

dvisc	0.0001388	Pa×s	756.13	Joback Method
dvisc	0.0001868	Pa×s	695.80	Joback Method
dvisc	0.0002659	Pa×s	635.48	Joback Method
dvisc	0.0004077	Pa×s	575.15	Joback Method
dvisc	0.0006909	Pa×s	514.82	Joback Method
dvisc	0.0013470	Pa×s	454.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339877&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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