1,2-Cyclohexanedicarboxylic acid, butyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C20H28O6/c1-4-5-13-25-19(21)14-9-6-7-10-15(14)20(22)26-18-16(23-2)11-8-1

InchiKey: LKKZWDBWXMCOIG-UHFFFAOYSA-N

Formula: C20H28O6

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-450.43	kJ/mol	Joback Method
hf	-962.60	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	86.97	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.759		Crippen Method
mcvol	284.660	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2602.00		NIST Webbook
tb	905.94	K	Joback Method
tc	1125.31	K	Joback Method
tf	558.54	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.22	J/mol×K	905.94	Joback Method
cpg	993.57	J/mol×K	1088.75	Joback Method
cpg	985.28	J/mol×K	1052.19	Joback Method
cpg	975.18	J/mol×K	1015.63	Joback Method
cpg	963.29	J/mol×K	979.06	Joback Method
cpg	949.63	J/mol×K	942.50	Joback Method
cpg	1000.05	J/mol×K	1125.31	Joback Method
dvisc	0.0000423	Pa×s	905.94	Joback Method

dvisc	0.0000530	Pa×s	848.04	Joback Method
dvisc	0.0000686	Pa×s	790.14	Joback Method
dvisc	0.0000924	Pa×s	732.24	Joback Method
dvisc	0.0001311	Pa×s	674.34	Joback Method
dvisc	0.0001986	Pa×s	616.44	Joback Method
dvisc	0.0003278	Pa×s	558.54	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=U339932&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