1,2-Cyclohexanedicarboxylic acid, butyl 3,5-dimethylcyclohexyl ester

Inchi: InChI=1S/C20H34O4/c1-4-5-10-23-19(21)17-8-6-7-9-18(17)20(22)24-16-12-14(2)11-15(3

InchiKey: JNPPGIMVNNVHHV-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-324.55	kJ/mol	Joback Method
hf	-898.11	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.504		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2273.00		NIST Webbook
tb	834.67	K	Joback Method
tc	1048.07	K	Joback Method
tf	461.52	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.20	J/mol×K	834.67	Joback Method
cpg	1061.03	J/mol×K	1012.51	Joback Method
cpg	1047.04	J/mol×K	976.94	Joback Method
cpg	1031.26	J/mol×K	941.37	Joback Method
cpg	1013.71	J/mol×K	905.80	Joback Method
cpg	994.36	J/mol×K	870.24	Joback Method
cpg	1073.26	J/mol×K	1048.07	Joback Method
dvisc	0.0001214	Pa×s	834.67	Joback Method
dvisc	0.0001536	Pa×s	772.48	Joback Method

dvisc	0.0002024	Pa×s	710.29	Joback Method
dvisc	0.0002812	Pa×s	648.10	Joback Method
dvisc	0.0004191	Pa×s	585.90	Joback Method
dvisc	0.0006866	Pa×s	523.71	Joback Method
dvisc	0.0012850	Pa×s	461.52	Joback Method

Sources

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=U339847&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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