Cyclohexanecarboxylic acid, 4-methoxy-, butyl ester

Inchi: InChI=1S/C12H22O3/c1-3-4-9-15-12(13)10-5-7-11(14-2)8-6-10/h10-11H,3-9H2,1-2H3
InchiKey: RWMKKRUZLLRKQE-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: CCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
gf	-272.02	kJ/mol	Joback Method
hf	-634.05	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.535		Crippen Method
mcvol	182.390	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1542.00		NIST Webbook
tb	587.55	K	Joback Method
tc	785.10	K	Joback Method
tf	322.53	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.16	J/mol×K	587.55	Joback Method
cpg	503.22	J/mol×K	620.48	Joback Method
cpg	521.36	J/mol×K	653.40	Joback Method
cpg	538.58	J/mol×K	686.33	Joback Method
cpg	554.87	J/mol×K	719.25	Joback Method
cpg	570.24	J/mol×K	752.18	Joback Method
cpg	584.69	J/mol×K	785.10	Joback Method
dvisc	0.0022926	Pa×s	322.53	Joback Method
dvisc	0.0011673	Pa×s	366.70	Joback Method

dvisc	0.0006872	Pa×s	410.87	Joback Method
dvisc	0.0004484	Pa×s	455.04	Joback Method
dvisc	0.0003155	Pa×s	499.21	Joback Method
dvisc	0.0002351	Pa×s	543.38	Joback Method
dvisc	0.0001831	Pa×s	587.55	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=U406191&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