Cyclohexanecarboxylic acid, 1-butyl-, methyl ester

Other names: 1-Butylcyclohexanecarboxylic acid methyl ester
Inchi: InChI=1S/C12H22O2/c1-3-4-8-12(11(13)14-2)9-6-5-7-10-12/h3-10H2,1-2H3
InchiKey: HFYNTJSQXRBKTO-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CCCCC1(C(=O)OC)CCCCC1
Mol. weight [g/mol]: 198.30
CAS: 7362-81-4

Physical Properties

Property code	Value	Unit	Source
gf	-164.80	kJ/mol	Joback Method
hf	-466.25	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	50.74	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.300		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	570.04	K	Joback Method
tc	777.13	K	Joback Method
tf	328.44	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.18	J/mol×K	570.04	Joback Method
cpg	472.10	J/mol×K	604.56	Joback Method
cpg	489.98	J/mol×K	639.07	Joback Method
cpg	506.93	J/mol×K	673.59	Joback Method
cpg	523.03	J/mol×K	708.10	Joback Method
cpg	538.38	J/mol×K	742.62	Joback Method

cpg	553.07	J/mol×K	777.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7362814&Units=SI

Legend

cpg:	Ideal gas heat capacity
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