Carbonic acid, butyl cyclohexylmethyl ester

Inchi: InChI=1S/C12H22O3/c1-2-3-9-14-12(13)15-10-11-7-5-4-6-8-11/h11H,2-10H2,1H3
InchiKey: JLIOMAHBSOWBDM-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: CCCCOC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
gf	-264.31	kJ/mol	Joback Method
hf	-613.71	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.520		Crippen Method
mcvol	182.390	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1531.00		NIST Webbook
tb	592.22	K	Joback Method
tc	789.92	K	Joback Method
tf	326.77	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.09	J/mol×K	592.22	Joback Method
cpg	501.71	J/mol×K	625.17	Joback Method
cpg	519.41	J/mol×K	658.12	Joback Method
cpg	536.19	J/mol×K	691.07	Joback Method
cpg	552.05	J/mol×K	724.02	Joback Method
cpg	566.99	J/mol×K	756.97	Joback Method
cpg	581.03	J/mol×K	789.92	Joback Method
dvisc	0.0026804	Pa×s	326.77	Joback Method
dvisc	0.0012663	Pa×s	371.01	Joback Method

dvisc	0.0007018	Pa×s	415.25	Joback Method
dvisc	0.0004358	Pa×s	459.50	Joback Method
dvisc	0.0002942	Pa×s	503.74	Joback Method
dvisc	0.0002117	Pa×s	547.98	Joback Method
dvisc	0.0001600	Pa×s	592.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357845&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