Carbonic acid, isobutyl cyclohexyl ester

Inchi: InChI=1S/C11H20O3/c1-9(2)8-13-11(12)14-10-6-4-3-5-7-10/h9-10H,3-8H2,1-2H3
InchiKey: JJVYAOKOEVWOFU-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CC(C)COC(=O)OC1CCCCC1
Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-275.17	kJ/mol	Joback Method
hf	-598.35	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	51.69	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.128		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1364.00		NIST Webbook
tb	568.90	K	Joback Method
tc	773.52	K	Joback Method
tf	300.50	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.18	J/mol×K	568.90	Joback Method
cpg	450.70	J/mol×K	603.00	Joback Method
cpg	468.28	J/mol×K	637.11	Joback Method
cpg	484.94	J/mol×K	671.21	Joback Method
cpg	500.68	J/mol×K	705.31	Joback Method
cpg	515.49	J/mol×K	739.42	Joback Method
cpg	529.38	J/mol×K	773.52	Joback Method
dvisc	0.0038404	Pa×s	300.50	Joback Method
dvisc	0.0016222	Pa×s	345.23	Joback Method

dvisc	0.0008350	Pa×s	389.97	Joback Method
dvisc	0.0004928	Pa×s	434.70	Joback Method
dvisc	0.0003209	Pa×s	479.43	Joback Method
dvisc	0.0002248	Pa×s	524.17	Joback Method
dvisc	0.0001666	Pa×s	568.90	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=U357827&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