Carbonic acid, neopentyl phenyl ester

Inchi: InChI=1S/C12H16O3/c1-12(2,3)9-14-11(13)15-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey: NPZHSLKOUUVCQB-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: CC(C)(C)COC(=O)Oc1ccccc1
Mol. weight [g/mol]: 208.25
CAS: 13183-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-173.51	kJ/mol	Joback Method
hf	-440.25	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	54.85	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.248		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1431.00		NIST Webbook
tb	596.12	K	Joback Method
tc	812.11	K	Joback Method
tf	348.23	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.01	J/mol×K	596.12	Joback Method
cpg	438.67	J/mol×K	632.12	Joback Method
cpg	453.34	J/mol×K	668.12	Joback Method
cpg	467.05	J/mol×K	704.12	Joback Method
cpg	479.83	J/mol×K	740.12	Joback Method
cpg	491.72	J/mol×K	776.11	Joback Method
cpg	502.73	J/mol×K	812.11	Joback Method
dvisc	0.0018343	Pa×s	348.23	Joback Method

dvisc	0.0009372	Pa×s	389.55	Joback Method
dvisc	0.0005447	Pa×s	430.86	Joback Method
dvisc	0.0003481	Pa×s	472.18	Joback Method
dvisc	0.0002391	Pa×s	513.49	Joback Method
dvisc	0.0001737	Pa×s	554.81	Joback Method
dvisc	0.0001319	Pa×s	596.12	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=C13183192&Units=SI

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