Carbonic acid, neopentyl 3,5-dimethylphenyl ester

Inchi: InChI=1S/C14H20O3/c1-10-6-11(2)8-12(7-10)17-13(15)16-9-14(3,4)5/h6-8H,9H2,1-5H3
InchiKey: FKHNWXTZUPREQT-UHFFFAOYSA-N
Formula: C14H20O3
SMILES: Cc1cc(C)cc(OC(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-175.93	kJ/mol	Joback Method
hf	-504.47	kJ/mol	Joback Method
hfus	21.84	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.865		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1622.00		NIST Webbook
tb	651.84	K	Joback Method
tc	862.62	K	Joback Method
tf	395.81	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.45	J/mol×K	651.84	Joback Method
cpg	539.72	J/mol×K	686.97	Joback Method
cpg	555.02	J/mol×K	722.10	Joback Method
cpg	569.37	J/mol×K	757.23	Joback Method
cpg	582.80	J/mol×K	792.36	Joback Method
cpg	595.33	J/mol×K	827.49	Joback Method
cpg	606.97	J/mol×K	862.62	Joback Method
dvisc	0.0009790	Pa×s	395.81	Joback Method
dvisc	0.0005574	Pa×s	438.48	Joback Method

dvisc	0.0003508	Pa×s	481.15	Joback Method
dvisc	0.0002380	Pa×s	523.83	Joback Method
dvisc	0.0001712	Pa×s	566.50	Joback Method
dvisc	0.0001290	Pa×s	609.17	Joback Method
dvisc	0.0001008	Pa×s	651.84	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=U357861&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