Carbonic acid, neopentyl 4-methoxyphenyl ester

Inchi: InChI=1S/C13H18O4/c1-13(2,3)9-16-12(14)17-11-7-5-10(15-4)6-8-11/h5-8H,9H2,1-4H3
InchiKey: SFIMQWQPJSPVFB-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: COc1ccc(OC(=O)OCC(C)(C)C)cc1
Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-279.72	kJ/mol	Joback Method
hf	-604.58	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	60.15	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.257		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1695.00		NIST Webbook
tb	646.40	K	Joback Method
tc	857.34	K	Joback Method
tf	394.25	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.95	J/mol×K	646.40	Joback Method
cpg	514.56	J/mol×K	681.56	Joback Method
cpg	529.23	J/mol×K	716.71	Joback Method
cpg	542.97	J/mol×K	751.87	Joback Method
cpg	555.78	J/mol×K	787.03	Joback Method
cpg	567.69	J/mol×K	822.19	Joback Method
cpg	578.71	J/mol×K	857.34	Joback Method
dvisc	0.0009322	Pa×s	394.25	Joback Method

dvisc	0.0005225	Pa×s	436.27	Joback Method
dvisc	0.0003242	Pa×s	478.30	Joback Method
dvisc	0.0002173	Pa×s	520.33	Joback Method
dvisc	0.0001546	Pa×s	562.35	Joback Method
dvisc	0.0001153	Pa×s	604.38	Joback Method
dvisc	0.0000894	Pa×s	646.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357862&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