Carbonic acid, neopentyl 3-methylphenyl ester

Inchi: InChI=1S/C13H18O3/c1-10-6-5-7-11(8-10)16-12(14)15-9-13(2,3)4/h5-8H,9H2,1-4H3
InchiKey: OMEIGROPJSTJFR-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: Cc1cccc(OC(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-174.72	kJ/mol	Joback Method
hf	-472.36	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	57.74	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.557		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	623.98	K	Joback Method
tc	837.28	K	Joback Method
tf	372.02	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.53	J/mol×K	623.98	Joback Method
cpg	488.51	J/mol×K	659.53	Joback Method
cpg	503.52	J/mol×K	695.08	Joback Method
cpg	517.57	J/mol×K	730.63	Joback Method
cpg	530.70	J/mol×K	766.18	Joback Method
cpg	542.93	J/mol×K	801.73	Joback Method
cpg	554.30	J/mol×K	837.28	Joback Method
dvisc	0.0013196	Pa×s	372.02	Joback Method

dvisc	0.0007150	Pa×s	414.01	Joback Method
dvisc	0.0004337	Pa×s	456.01	Joback Method
dvisc	0.0002862	Pa×s	498.00	Joback Method
dvisc	0.0002015	Pa×s	539.99	Joback Method
dvisc	0.0001492	Pa×s	581.99	Joback Method
dvisc	0.0001151	Pa×s	623.98	Joback Method

Sources

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=U357859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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