

tert-Butyl phenyl carbonate

Other names:	t-Butyl phenyl carbonate Carbonic acid, 1,1-dimethylethyl phenyl ester Carbonic acid 1,1-dimethylethyl ester
Inchi:	InChI=1S/C11H14O3/c1-11(2,3)14-10(12)13-9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	UXWVQHXXKOGTSY-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CC(C)(C)OC(=O)Oc1ccccc1
Mol. weight [g/mol]:	194.23
CAS:	6627-89-0

Physical Properties

Property code	Value	Unit	Source
gf	-181.93	kJ/mol	Joback Method
hf	-419.61	kJ/mol	Joback Method
hfus	14.85	kJ/mol	Joback Method
hvap	67.60 ± 0.60	kJ/mol	NIST Webbook
log10ws	-3.22		Crippen Method
logp	3.000		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	573.24	K	Joback Method
tc	793.08	K	Joback Method
tf	336.96	K	Joback Method
vc	0.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.61	J/mol×K	573.24	Joback Method
cpg	389.62	J/mol×K	609.88	Joback Method
cpg	403.67	J/mol×K	646.52	Joback Method
cpg	416.79	J/mol×K	683.16	Joback Method
cpg	429.01	J/mol×K	719.80	Joback Method
cpg	440.35	J/mol×K	756.44	Joback Method

cpg	450.86	J/molxK	793.08	Joback Method
dvisc	0.0019508	Paxs	336.96	Joback Method
dvisc	0.0010129	Paxs	376.34	Joback Method
dvisc	0.0005955	Paxs	415.72	Joback Method
dvisc	0.0003838	Paxs	455.10	Joback Method
dvisc	0.0002653	Paxs	494.48	Joback Method
dvisc	0.0001936	Paxs	533.86	Joback Method
dvisc	0.0001476	Paxs	573.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.70	K	0.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6627890&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
tb:	Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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