Peroxybenzoic acid, tert-butyl ester

Other names: tert-butyl perbenzoate
tert-Butyl peroxybenzoate
Inchi: InChI=1S/C11H14O3/c1-11(2,3)14-13-10(12)9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey: GJBRNHKUVLOCEB-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(C)(C)OOC(=O)c1ccccc1
Mol. weight [g/mol]: 194.23
CAS: 614-45-9

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	52.63	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.574		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.61	J/mol×K	573.24	Joback Method
cpg	440.35	J/mol×K	756.44	Joback Method
cpg	429.01	J/mol×K	719.80	Joback Method
cpg	416.79	J/mol×K	683.16	Joback Method
cpg	403.67	J/mol×K	646.52	Joback Method
cpg	389.62	J/mol×K	609.88	Joback Method
cpg	450.86	J/mol×K	793.08	Joback Method

dvisc	0.0001476	Pa×s	573.24	Joback Method
dvisc	0.0001936	Pa×s	533.86	Joback Method
dvisc	0.0002653	Pa×s	494.48	Joback Method
dvisc	0.0003838	Pa×s	455.10	Joback Method
dvisc	0.0005955	Pa×s	415.72	Joback Method
dvisc	0.0010129	Pa×s	376.34	Joback Method
dvisc	0.0019508	Pa×s	336.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.70	K	0.03	NIST Webbook

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=C614459&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume