

Peroxycarbonic acid, oo-tert-butyl isopropyl ester

Other names:	O,O-tert-butyl isopropyl monoperoxy carbonate
Inchi:	InChI=1S/C8H16O4/c1-6(2)10-7(9)11-12-8(3,4)5/h6H,1-5H3
InchiKey:	KDGNCLDCOVTOCS-UHFFFAOYSA-N
Formula:	C8H16O4
SMILES:	CC(C)OC(=O)OOC(C)(C)C
Mol. weight [g/mol]:	176.21
CAS:	2372-21-6

Physical Properties

Property code	Value	Unit	Source
gf	-427.04	kJ/mol	Joback Method
hf	-731.72	kJ/mol	Joback Method
hfus	10.70	kJ/mol	Joback Method
hvap	45.69	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.278		Crippen Method
mcvol	142.760	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
tb	499.90	K	Joback Method
tc	688.09	K	Joback Method
tf	283.96	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.35	J/molxK	499.90	Joback Method
cpg	344.57	J/molxK	531.26	Joback Method
cpg	357.28	J/molxK	562.63	Joback Method
cpg	369.46	J/molxK	593.99	Joback Method
cpg	381.12	J/molxK	625.36	Joback Method
cpg	392.25	J/molxK	656.72	Joback Method
cpg	402.84	J/molxK	688.09	Joback Method
dvisc	0.0031632	Paxs	283.96	Joback Method

dvisc	0.0014584	Paxs	319.95	Joback Method
dvisc	0.0007864	Paxs	355.94	Joback Method
dvisc	0.0004749	Paxs	391.93	Joback Method
dvisc	0.0003122	Paxs	427.92	Joback Method
dvisc	0.0002191	Paxs	463.91	Joback Method
dvisc	0.0001618	Paxs	499.90	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=C2372216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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