

di-tert-butyl sec-butyldiene diperoxide

Other names:	2,2-Bis(tert-butylperoxy) butane
Inchi:	InChI=1S/C12H26O4/c1-9-12(8,15-13-10(2,3)4)16-14-11(5,6)7/h9H2,1-8H3
InchiKey:	HQOVXPHOJANJBR-UHFFFAOYSA-N
Formula:	C12H26O4
SMILES:	CCC(C)(OOC(C)(C)C)OOC(C)(C)C
Mol. weight [g/mol]:	234.33
CAS:	2167-23-9

Physical Properties

Property code	Value	Unit	Source
gf	-361.32	kJ/mol	Joback Method
hf	-846.14	kJ/mol	Joback Method
hfus	9.35	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.606		Crippen Method
mcvol	203.420	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
tb	553.95	K	Joback Method
tc	741.20	K	Joback Method
tf	321.18	K	Joback Method
vc	0.747	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.13	J/molxK	553.95	Joback Method
cpg	548.71	J/molxK	585.16	Joback Method
cpg	566.37	J/molxK	616.37	Joback Method
cpg	583.12	J/molxK	647.57	Joback Method
cpg	598.99	J/molxK	678.78	Joback Method
cpg	614.01	J/molxK	709.99	Joback Method
cpg	628.19	J/molxK	741.20	Joback Method
dvisc	0.0023173	Paxs	321.18	Joback Method

dvisc	0.0009523	Paxs	359.98	Joback Method
dvisc	0.0004652	Paxs	398.77	Joback Method
dvisc	0.0002581	Paxs	437.57	Joback Method
dvisc	0.0001576	Paxs	476.36	Joback Method
dvisc	0.0001036	Paxs	515.16	Joback Method
dvisc	0.0000723	Paxs	553.95	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=C2167239&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	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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