

Peroxide, bis(1,1-dimethylethyl)

Other names:	(tert-C4H9O)2 Bis(1,1-dimethylethyl) peroxide Bis(tert-butyl) peroxide Cadox Cadox TBP DTBP Di-t-butyl peroxide Di-tert-butyl peroxyde Di-tert-butylperoxid Di-tertiary-butyl peroxide Interox DTB Kayabutyl D NSC 673 Perbutyl D Perossido di butile terziario Peroxide, bis-tert-butyl- Peroxide, tert-butyl- Peroxyde de butyle tertiaire Trigonox B t-Butyl peroxide t-butyl peroxide bis(1,1-di-methylethyl)peroxide tert-Butyl peroxide
Inchi:	InChI=1S/C8H18O2/c1-7(2,3)9-10-8(4,5)6/h1-6H3
InchiKey:	LSXWFXONGKSEMY-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CC(C)(C)OOC(C)(C)C
Mol. weight [g/mol]:	146.23
CAS:	110-05-4

Physical Properties

Property code	Value	Unit	Source
af	0.4440		Cheméo Relay (1.0)
chl	-5339.80 ± 1.60	kJ/mol	NIST Webbook
chl	-5326.00	kJ/mol	NIST Webbook
chl	-5334.60	kJ/mol	NIST Webbook
chl	-5339.60 ± 0.80	kJ/mol	NIST Webbook

chl	-5336.30	kJ/mol	NIST Webbook
gf	-187.84	kJ/mol	Joback Method
hf	-341.00	kJ/mol	NIST Webbook
hf	-343.00	kJ/mol	NIST Webbook
hf	-340.80	kJ/mol	NIST Webbook
hfl	-381.00	kJ/mol	NIST Webbook
hfl	-385.00	kJ/mol	NIST Webbook
hfl	-380.80 ± 2.00	kJ/mol	NIST Webbook
hfus	4.02	kJ/mol	Joback Method
hvap	43.09	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
log10ws	-2.27		Cheméo Relay (1.0)
logp	2.532		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
tb	382.70	K	NIST Webbook
tc	564.85	K	Cheméo Relay (1.0)
tf	302.58	K	Cheméo Relay (1.0)
vc	0.557	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.25	J/mol×K	420.82	Joback Method
cpg	301.47	J/mol×K	451.79	Joback Method
cpg	315.98	J/mol×K	482.76	Joback Method
cpg	329.80	J/mol×K	513.74	Joback Method
cpg	342.94	J/mol×K	544.71	Joback Method
cpg	355.43	J/mol×K	575.68	Joback Method
cpg	367.29	J/mol×K	606.65	Joback Method
dvisc	0.0075653	Pa×s	229.22	Joback Method
dvisc	0.0029132	Pa×s	261.15	Joback Method
dvisc	0.0013811	Pa×s	293.09	Joback Method
dvisc	0.0007582	Pa×s	325.02	Joback Method
dvisc	0.0004634	Pa×s	356.95	Joback Method
dvisc	0.0003070	Pa×s	388.89	Joback Method
dvisc	0.0002166	Pa×s	420.82	Joback Method
hvapt	37.00	kJ/mol	333.00	NIST Webbook
hvapt	32.00	kJ/mol	278.50	NIST Webbook
hvapt	31.00	kJ/mol	328.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	9.64980e+00
Coeff. B	-2.14376e+03
Coeff. C	-5.29490e+01
Temperature range (K), min.	281.93
Temperature range (K), max.	547.09

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C110054&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/13-383-2/Peroxide-bis-1-1-dimethylethyl.pdf>

Generated by Cheméo on 2026-07-21 14:18:50.008685546 +0000 UTC m=+154625.850570916.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.