

Peroxide, diethyl

Other names:	Ethyl peroxide Diethyl peroxide
Inchi:	InChI=1S/C4H10O2/c1-3-5-6-4-2/h3-4H2,1-2H3
InchiKey:	RHMZKSWPMYAOAZ-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CCOCC
Mol. weight [g/mol]:	90.12
CAS:	628-37-5

Physical Properties

Property code	Value	Unit	Source
chl	-2771.00	kJ/mol	NIST Webbook
chl	-2697.90 ± 0.84	kJ/mol	NIST Webbook
chl	-2780.00 ± 1.00	kJ/mol	NIST Webbook
gf	-327.57	kJ/mol	Joback Method
hf	-200.00	kJ/mol	NIST Webbook
hf	-280.00	kJ/mol	NIST Webbook
hf	-193.00	kJ/mol	NIST Webbook
hfl	-223.00	kJ/mol	NIST Webbook
hfl	-233.00	kJ/mol	NIST Webbook
hfus	10.48	kJ/mol	Joback Method
hvap	30.00	kJ/mol	NIST Webbook
hvap	30.50	kJ/mol	NIST Webbook
hvap	31.00	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
log10ws	-0.66		Crippen Method
logp	0.974		Crippen Method
mvol	78.960	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	349.14	K	Joback Method
tc	523.60	K	Joback Method
tf	177.17	K	Joback Method
vc	0.285	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.57	J/molxK	349.14	Joback Method
cpg	133.80	J/molxK	378.22	Joback Method
cpg	140.82	J/molxK	407.29	Joback Method
cpg	147.63	J/molxK	436.37	Joback Method
cpg	154.23	J/molxK	465.45	Joback Method
cpg	160.62	J/molxK	494.52	Joback Method
cpg	166.78	J/molxK	523.60	Joback Method
dvisc	0.0023057	Paxs	205.83	Joback Method
dvisc	0.0053747	Paxs	177.17	Joback Method
dvisc	0.0012165	Paxs	234.49	Joback Method
dvisc	0.0007377	Paxs	263.15	Joback Method
dvisc	0.0004936	Paxs	291.82	Joback Method
dvisc	0.0003548	Paxs	320.48	Joback Method
dvisc	0.0002693	Paxs	349.14	Joback Method
hvapt	29.00	kJ/mol	293.00	NIST Webbook
hvapt	29.00	kJ/mol	253.00	NIST Webbook

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=C628375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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