

1,4-Epoxyaphthalene, 1,4-dihydro-

Other names:	1,4-Dihydro-1,4-epoxyaphthalene 1,4-Dihydronaphthalene-1,4-oxide 1,4-Dihydronaphthalene-1,4-endo-oxide 1,4-Epoxy-1,4-dihydronaphthalene 7-Oxabenzonorbornadiene
Inchi:	InChI=1S/C10H8O/c1-2-4-8-7(3-1)9-5-6-10(8)11-9/h1-6,9-10H
InchiKey:	JWCGDNHAPBZVHD-UHFFFAOYSA-N
Formula:	C10H8O
SMILES:	C1=CC2OC1c1cccc12
Mol. weight [g/mol]:	144.17
CAS:	573-57-9

Physical Properties

Property code	Value	Unit	Source
chs	-5140.50	kJ/mol	NIST Webbook
gf	213.54	kJ/mol	Joback Method
hf	52.87	kJ/mol	Joback Method
hfs	62.10 ± 5.80	kJ/mol	NIST Webbook
hfus	22.88	kJ/mol	Joback Method
hvap	45.25	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.369		Crippen Method
mvol	107.850	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	495.18	K	Joback Method
tc	728.70	K	Joback Method
tf	308.13	K	Joback Method
vc	0.416	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.44	J/mol×K	495.18	Joback Method
cpg	300.16	J/mol×K	689.78	Joback Method

cpg	290.44	J/molxK	650.86	Joback Method
cpg	279.83	J/molxK	611.94	Joback Method
cpg	268.20	J/molxK	573.02	Joback Method
cpg	255.44	J/molxK	534.10	Joback Method
cpg	309.10	J/molxK	728.70	Joback Method
dvisc	0.0010840	Paxs	495.18	Joback Method
dvisc	0.0011018	Paxs	464.00	Joback Method
dvisc	0.0011226	Paxs	432.83	Joback Method
dvisc	0.0011470	Paxs	401.65	Joback Method
dvisc	0.0011763	Paxs	370.48	Joback Method
dvisc	0.0012119	Paxs	339.31	Joback Method
dvisc	0.0012562	Paxs	308.13	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=C573579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid 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
hfs:	Solid phase 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
mccvol:	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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