1,2,3,4-Tetrahydro-1-hydroperoxynaphthalene

Inchi: InChI=1S/C10H12O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h1-2,4,6,10-11H,3,5,7H2
InchiKey: YWBMNCRJFZGXJY-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: OOC1CCCc2ccccc21
Mol. weight [g/mol]: 164.20
CAS: 26447-24-5

Physical Properties

Property code	Value	Unit	Source
chs	-5468.50 ± 8.40	kJ/mol	NIST Webbook
chs	-5462.60	kJ/mol	NIST Webbook
gf	-57.07	kJ/mol	Joback Method
hf	-242.48	kJ/mol	Joback Method
hfs	-187.40 ± 5.40	kJ/mol	NIST Webbook
hfus	16.62	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.554		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	585.47	K	Joback Method
tc	797.79	K	Joback Method
tf	338.87	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.32	J/mol×K	585.47	Joback Method
cpg	334.62	J/mol×K	620.86	Joback Method
cpg	347.09	J/mol×K	656.24	Joback Method
cpg	358.77	J/mol×K	691.63	Joback Method
cpg	369.69	J/mol×K	727.02	Joback Method
cpg	379.89	J/mol×K	762.41	Joback Method

cpg	389.40	J/mol×K	797.79	Joback Method
dvisc	0.0041419	Pa×s	338.87	Joback Method
dvisc	0.0017090	Pa×s	379.97	Joback Method
dvisc	0.0008382	Pa×s	421.07	Joback Method
dvisc	0.0004666	Pa×s	462.17	Joback Method
dvisc	0.0002858	Pa×s	503.27	Joback Method
dvisc	0.0001885	Pa×s	544.37	Joback Method
dvisc	0.0001319	Pa×s	585.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26447245&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume