1H,3H-Naphtho[1,8-cd]pyran-1-one

Other names:	Peri-Naphthalide
	Naphthalid
	Naphthalide
	1-Naphthalenecarboxylic acid, 8-(hydroxymethyl)-, «delta»-lactone
	1-Naphthoic acid, 8-(hydroxymethyl)-, «delta»-lactone
	1,8-Naphthalide
Inchi:	InChI=1S/C12H8O2/c13-12-10-6-2-4-8-3-1-5-9(7-14-12)11(8)10/h1-6H,7H2
InchiKey:	UKOVZLWSUZKTRL-UHFFFAOYSA-N
Formula:	C12H8O2
SMILES:	O=C1OCc2cccc3cccc1c23
Mol. weight [g/mol]:	184.19
CAS:	518-86-5

Physical Properties

Property code	Value	Unit	Source
gf	109.71	kJ/mol	Joback Method
hf	-62.91	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.510		Crippen Method
mcvol	133.300	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1828.00		NIST Webbook
tb	635.76	K	Joback Method
tc	896.34	K	Joback Method
tf	426.13	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.53	J/mol×K	635.76	Joback Method
cpg	343.79	J/mol×K	679.19	Joback Method

cpg	355.97	J/mol×K	722.62	Joback Method
cpg	367.18	J/mol×K	766.05	Joback Method
cpg	377.51	J/mol×K	809.48	Joback Method
cpg	387.04	J/mol×K	852.91	Joback Method
cpg	395.89	J/mol×K	896.34	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=C518865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume