1H-Phenalen-1-one

Other names:	Phenalen-1-one
	Perinaphthenone
	Phenalenone
	7-Perinaphthenone
	Perinaphthanone
Inchi:	InChI=1S/C13H8O/c14-12-8-7-10-4-1-3-9-5-2-6-11(12)13(9)10/h1-8H
InchiKey:	WWBGWPHHLRSTFI-UHFFFAOYSA-N
Formula:	C13H8O
SMILES:	O=C1C=Cc2cccc3cccc1c23
Mol. weight [g/mol]:	180.20
CAS:	548-39-0

Physical Properties

Property code	Value	Unit	Source
gf	234.21	kJ/mol	Joback Method
hf	106.23	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
ie	8.20 ± 0.04	eV	NIST Webbook
log10ws	-4.24		Crippen Method
logp	3.049		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	320.74		NIST Webbook
rinpol	317.00		NIST Webbook
rinpol	317.42		NIST Webbook
rinpol	317.42		NIST Webbook
rinpol	1751.00		NIST Webbook
rinpol	319.80		NIST Webbook
rinpol	319.70		NIST Webbook
rinpol	320.74		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	630.85	K	Joback Method
tc	892.23	K	Joback Method
tf	411.59	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.47	J/mol×K	848.67	Joback Method
cpg	329.11	J/mol×K	630.85	Joback Method
cpg	342.59	J/mol×K	674.41	Joback Method
cpg	354.95	J/mol×K	717.98	Joback Method
cpg	366.32	J/mol×K	761.54	Joback Method
cpg	376.79	J/mol×K	805.11	Joback Method
cpg	395.47	J/mol×K	892.23	Joback Method
hsubt	97.20 ± 2.50	kJ/mol	337.00	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C548390&Units=SI

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
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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

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