9-Phenanthrenol

Other names:	9-Phenanthrol
	9-Hydroxyphenanthrene
	phenanthren-9-ol
Inchi:	InChI=1S/C14H10O/c15-14-9-10-5-1-2-6-11(10)12-7-3-4-8-13(12)14/h1-9,15H
InchiKey:	DZKIUEHLEXLYKM-UHFFFAOYSA-N
Formula:	C14H10O
SMILES:	Oc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]:	194.23
CAS:	484-17-3

Physical Properties

Property code	Value	Unit	Source
gf	228.46	kJ/mol	Joback Method
hf	97.60	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.699		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	669.96	K	Joback Method
tc	932.17	K	Joback Method
tf	463.60	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.08	J/mol×K	669.96	Joback Method
cpg	393.60	J/mol×K	713.66	Joback Method
cpg	405.10	J/mol×K	757.36	Joback Method
cpg	415.82	J/mol×K	801.06	Joback Method

cpg	425.98	J/mol×K	844.77	Joback Method
cpg	435.80	J/mol×K	888.47	Joback Method
cpg	445.51	J/mol×K	932.17	Joback Method
dvisc	0.0006150	Pa×s	463.60	Joback Method
dvisc	0.0003636	Pa×s	497.99	Joback Method
dvisc	0.0002300	Pa×s	532.39	Joback Method
dvisc	0.0001539	Pa×s	566.78	Joback Method
dvisc	0.0001078	Pa×s	601.17	Joback Method
dvisc	0.0000784	Pa×s	635.57	Joback Method
dvisc	0.0000590	Pa×s	669.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C484173&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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