1,3,5,7-Cyclooctatetraene, 1-phenyl-

Other names: 1-phenyl-1,3,5,7-cyclo-octatetraene
Inchi: InChI=1S/C14H12/c1-2-5-9-13(10-6-3-1)14-11-7-4-8-12-14/h1-12H/b2-1-,3-1-,5-2-,6-3-,9
InchiKey: GONKWCNPVBWYRY-ZACRBJJOSA-N
Formula: C14H12
SMILES: C1=CC=CC(c2ccccc2)=CC=C1
Mol. weight [g/mol]: 180.25
CAS: 4603-00-3

Physical Properties

Property code	Value	Unit	Source
gf	297.58	kJ/mol	Joback Method
hf	186.23	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.752		Crippen Method
mcvol	156.300	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	279.98		NIST Webbook
rinpol	279.98		NIST Webbook
tb	580.78	K	Joback Method
tc	841.19	K	Joback Method
tf	294.10	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.44	J/mol×K	580.78	Joback Method
cpg	373.01	J/mol×K	624.18	Joback Method
cpg	390.04	J/mol×K	667.58	Joback Method
cpg	405.58	J/mol×K	710.99	Joback Method
cpg	419.72	J/mol×K	754.39	Joback Method
cpg	432.53	J/mol×K	797.79	Joback Method

cpg	444.08	J/mol×K	841.19	Joback Method
dvisc	0.0032891	Pa×s	294.10	Joback Method
dvisc	0.0012556	Pa×s	341.88	Joback Method
dvisc	0.0006070	Pa×s	389.66	Joback Method
dvisc	0.0003439	Pa×s	437.44	Joback Method
dvisc	0.0002180	Pa×s	485.22	Joback Method
dvisc	0.0001499	Pa×s	533.00	Joback Method
dvisc	0.0001096	Pa×s	580.78	Joback Method

Sources

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=C4603003&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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