Phenanthrene, 2,4,5,7-tetramethyl-

Other names: 2,4,5,7-Tetramethylphenanthrene
Inchi: InChI=1S/C18H18/c1-11-7-13(3)17-15(9-11)5-6-16-10-12(2)8-14(4)18(16)17/h5-10H,1-4
InchiKey: BZXXZUAJRXKPOF-UHFFFAOYSA-N
Formula: C18H18
SMILES: Cc1cc(C)c2c(ccc3cc(C)cc(C)c32)c1
Mol. weight [g/mol]: 234.34
CAS: 7396-38-5

Physical Properties

Property code	Value	Unit	Source
chs	-9672.80 ± 2.30	kJ/mol	NIST Webbook
gf	378.24	kJ/mol	Joback Method
hf	130.00 ± 4.00	kJ/mol	NIST Webbook
hfs	16.00 ± 3.00	kJ/mol	NIST Webbook
hfus	28.51	kJ/mol	Joback Method
hsub	114.00	kJ/mol	NIST Webbook
hsub	114.00 ± 2.00	kJ/mol	NIST Webbook
hvap	64.53	kJ/mol	Joback Method
ie	7.80 ± 0.10	eV	NIST Webbook
log10ws	-6.98		Crippen Method
logp	5.227		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
tb	700.78	K	Joback Method
tc	937.00	K	Joback Method
tf	447.04	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.75	J/mol×K	700.78	Joback Method
cpg	602.50	J/mol×K	897.63	Joback Method
cpg	589.83	J/mol×K	858.26	Joback Method

cpg	576.42	J/mol×K	818.89	Joback Method
cpg	562.17	J/mol×K	779.52	Joback Method
cpg	546.98	J/mol×K	740.15	Joback Method
cpg	614.52	J/mol×K	937.00	Joback Method
dvisc	0.0003925	Pa×s	700.78	Joback Method
dvisc	0.0004376	Pa×s	658.49	Joback Method
dvisc	0.0004953	Pa×s	616.20	Joback Method
dvisc	0.0005708	Pa×s	573.91	Joback Method
dvisc	0.0006730	Pa×s	531.62	Joback Method
dvisc	0.0008162	Pa×s	489.33	Joback Method
dvisc	0.0010269	Pa×s	447.04	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=C7396385&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hsub: Enthalpy of sublimation at standard conditions
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume