

Phenanthrene, 4,5-dimethyl-

Other names:	4,5-Dimethylphenanthrene 4,5-methylphenanthrene
Inchi:	InChI=1S/C16H14/c1-11-5-3-7-13-9-10-14-8-4-6-12(2)16(14)15(11)13/h3-10H,1-2H3
InchiKey:	GWWHAAHVHHLOQW-UHFFFAOYSA-N
Formula:	C16H14
SMILES:	<chem>Cc1cccc2ccc3cccc(C)c3c12</chem>
Mol. weight [g/mol]:	206.28
CAS:	3674-69-9

Physical Properties

Property code	Value	Unit	Source
chs	-8385.90 ± 5.90	kJ/mol	NIST Webbook
gf	380.66	kJ/mol	Joback Method
hf	210.69	kJ/mol	Joback Method
hfs	88.90 ± 5.90	kJ/mol	NIST Webbook
hfus	24.11	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
ie	7.53 ± 0.04	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-6.03		Crippen Method
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1979.80		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	327.16		NIST Webbook
rinpol	327.16		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	645.06	K	Joback Method
tc	889.67	K	Joback Method
tf	399.46	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/molxK	645.06	Joback Method
cpg	445.30	J/molxK	685.83	Joback Method
cpg	459.74	J/molxK	726.60	Joback Method
cpg	473.15	J/molxK	767.36	Joback Method
cpg	485.63	J/molxK	808.13	Joback Method
cpg	497.31	J/molxK	848.90	Joback Method
cpg	508.31	J/molxK	889.67	Joback Method
dvisc	0.0012344	Paxs	399.46	Joback Method
dvisc	0.0009553	Paxs	440.39	Joback Method
dvisc	0.0007722	Paxs	481.33	Joback Method
dvisc	0.0006454	Paxs	522.26	Joback Method
dvisc	0.0005537	Paxs	563.19	Joback Method
dvisc	0.0004850	Paxs	604.13	Joback Method
dvisc	0.0004320	Paxs	645.06	Joback Method
hsubt	85.70	kJ/mol	383.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37543e+01
Coeff. B	-4.78678e+03
Coeff. C	-1.19348e+02
Temperature range (K), min.	474.80
Temperature range (K), max.	686.31

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C3674699&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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
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
pvap:	Vapor 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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