Chrysene, 5-methyl-

Other names: 5-Methylchrysene
Inchi: InChI=1S/C19H14/c1-13-12-15-7-3-4-8-16(15)18-11-10-14-6-2-5-9-17(14)19(13)18/h2-12
InchiKey: GOHBXWHNJHENRX-UHFFFAOYSA-N
Formula: C19H14
SMILES: Cc1cc2ccccc2c2ccc3ccccc3c12
Mol. weight [g/mol]: 242.31
CAS: 3697-24-3

Physical Properties

Property code	Value	Unit	Source
gf	512.57	kJ/mol	Joback Method
hf	339.84	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	67.07	kJ/mol	Joback Method
ie	7.40 ± 0.03	eV	NIST Webbook
log10ws	-6.59		Estimated Solubility Method
log10ws	-6.59		Aqueous Solubility Prediction Method
logp	5.455		Crippen Method
mcvol	196.430	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	420.40		NIST Webbook
rinpol	419.00		NIST Webbook
rinpol	419.00		NIST Webbook
rinpol	419.68		NIST Webbook
rinpol	419.68		NIST Webbook
rinpol	418.67		NIST Webbook
rinpol	420.01		NIST Webbook
rinpol	420.20		NIST Webbook
rinpol	418.67		NIST Webbook
tb	732.68	K	Joback Method
tc	990.82	K	Joback Method
tf	391.00 ± 1.00	K	NIST Webbook
tf	389.00 ± 4.00	K	NIST Webbook
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.11	J/mol×K	990.82	Joback Method
cpg	518.66	J/mol×K	732.68	Joback Method
cpg	533.84	J/mol×K	775.70	Joback Method
cpg	547.92	J/mol×K	818.73	Joback Method
cpg	561.09	J/mol×K	861.75	Joback Method
cpg	573.55	J/mol×K	904.77	Joback Method
cpg	585.49	J/mol×K	947.80	Joback Method
dvisc	0.0006851	Pa×s	732.68	Joback Method
dvisc	0.0016009	Pa×s	465.97	Joback Method
dvisc	0.0013067	Pa×s	510.42	Joback Method
dvisc	0.0011019	Pa×s	554.87	Joback Method
dvisc	0.0009529	Pa×s	599.33	Joback Method
dvisc	0.0008408	Pa×s	643.78	Joback Method
dvisc	0.0007540	Pa×s	688.23	Joback Method
hfust	19.00	kJ/mol	390.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40352e+01
Coeff. B	-5.59509e+03
Coeff. C	-1.44132e+02
Temperature range (K), min.	551.12
Temperature range (K), max.	785.50

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3697243&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hfust:	Enthalpy of fusion 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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