

2-Methylchrysene

Other names:	Chrysene, 2-methyl-
Inchi:	InChI=1S/C19H14/c1-13-6-9-17-15(12-13)8-11-18-16-5-3-2-4-14(16)7-10-19(17)18/h2-12
InchiKey:	PJVVBVYEMMJZCY-UHFFFAOYSA-N
Formula:	C19H14
SMILES:	<chem>Cc1ccc2c(ccc3c4ccccc4ccc23)c1</chem>
Mol. weight [g/mol]:	242.31
CAS:	3351-32-4

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	7.49 ± 0.03	eV	NIST Webbook
log10ws	-7.36		Crippen Method
logp	5.455		Crippen Method
mcvol	196.430	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	419.66		NIST Webbook
rinpol	415.11		NIST Webbook
rinpol	418.00		NIST Webbook
rinpol	418.80		NIST Webbook
rinpol	418.00		NIST Webbook
rinpol	418.80		NIST Webbook
rinpol	418.01		NIST Webbook
rinpol	419.70		NIST Webbook
rinpol	418.00		NIST Webbook
tb	732.68	K	Joback Method
tc	990.82	K	Joback Method
tf	465.97	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.66	J/molxK	732.68	Joback Method
cpg	585.49	J/molxK	947.80	Joback Method
cpg	573.55	J/molxK	904.77	Joback Method
cpg	561.09	J/molxK	861.75	Joback Method
cpg	547.92	J/molxK	818.73	Joback Method
cpg	533.84	J/molxK	775.70	Joback Method
cpg	597.11	J/molxK	990.82	Joback Method
dvisc	0.0006851	Paxs	732.68	Joback Method
dvisc	0.0007540	Paxs	688.23	Joback Method
dvisc	0.0008408	Paxs	643.78	Joback Method
dvisc	0.0009529	Paxs	599.33	Joback Method
dvisc	0.0011019	Paxs	554.87	Joback Method
dvisc	0.0013067	Paxs	510.42	Joback Method
dvisc	0.0016009	Paxs	465.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

- 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=C3351324&Units=SI>

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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