

Benz[a]anthracene, 2-methyl-

Other names:	2-Methylbenz[a]anthracene 2'-Methyl-1,2-benzanthracene
Inchi:	InChI=1S/C19H14/c1-13-6-7-14-8-9-17-11-15-4-2-3-5-16(15)12-19(17)18(14)10-13/h2-13
InchiKey:	XPRFYYVRSILJDC-UHFFFAOYSA-N
Formula:	C19H14
SMILES:	<chem>Cc1ccc2ccc3cc4ccccc4cc3c2c1</chem>
Mol. weight [g/mol]:	242.31
CAS:	2498-76-2

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	7.39	eV	NIST Webbook
ie	7.30 ± 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	414.10		NIST Webbook
rinpol	413.78		NIST Webbook
rinpol	413.78		NIST Webbook
rinpol	413.74		NIST Webbook
rinpol	413.78		NIST Webbook
tb	732.68	K	Joback Method
tc	990.82	K	Joback Method
tf	465.97	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	518.66	J/molxK	732.68	Joback Method
cpg	533.84	J/molxK	775.70	Joback Method
cpg	547.92	J/molxK	818.73	Joback Method
cpg	561.09	J/molxK	861.75	Joback Method
cpg	573.55	J/molxK	904.77	Joback Method
cpg	585.49	J/molxK	947.80	Joback Method
cpg	597.11	J/molxK	990.82	Joback Method
dvisc	0.0016009	Paxs	465.97	Joback Method
dvisc	0.0013067	Paxs	510.42	Joback Method
dvisc	0.0011019	Paxs	554.87	Joback Method
dvisc	0.0009529	Paxs	599.33	Joback Method
dvisc	0.0008408	Paxs	643.78	Joback Method
dvisc	0.0007540	Paxs	688.23	Joback Method
dvisc	0.0006851	Paxs	732.68	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=C2498762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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