Benz[a]anthracene, 10-methyl-

Other names: 10-Methylbenz[a]anthracene
7-Methyl-1,2-benzanthracene
Inchi: InChI=1S/C19H14/c1-13-6-7-15-11-16-9-8-14-4-2-3-5-18(14)19(16)12-17(15)10-13/h2-12
InchiKey: WUMGYHICFXGLAB-UHFFFAOYSA-N
Formula: C19H14
SMILES: Cc1ccc2cc3ccc4ccccc4c3cc2c1
Mol. weight [g/mol]: 242.31
CAS: 2381-15-9

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	7.30 ± 0.03	eV	NIST Webbook
ie	7.37	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	423.30		NIST Webbook
rinpol	423.30		NIST Webbook
rinpol	2611.00		NIST Webbook
rinpol	2575.00		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/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
cpg	597.11	J/mol×K	990.82	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
dvisc	0.0006851	Pa×s	732.68	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2381159&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
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