Anthracene, 2-(1,1-dimethylethyl)-

Other names: 2-(tert-butyl)anthracene
2-tert-Butylanthracene
Inchi: InChI=1S/C18H18/c1-18(2,3)17-9-8-15-10-13-6-4-5-7-14(13)11-16(15)12-17/h4-12H,1-3
InchiKey: WBPXZSIKOVBSAS-UHFFFAOYSA-N
Formula: C18H18
SMILES: CC(C)(C)c1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]: 234.34
CAS: 18801-00-8

Physical Properties

Property code	Value	Unit	Source
ea	0.50 ± 0.06	eV	NIST Webbook
gf	409.97	kJ/mol	Joback Method
hf	172.13	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.290		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
tb	682.61	K	Joback Method
tc	930.31	K	Joback Method
tf	411.90	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.09	J/mol×K	682.61	Joback Method
cpg	553.50	J/mol×K	723.89	Joback Method
cpg	569.54	J/mol×K	765.18	Joback Method
cpg	584.39	J/mol×K	806.46	Joback Method
cpg	598.21	J/mol×K	847.74	Joback Method
cpg	611.20	J/mol×K	889.02	Joback Method

cpg	623.51	J/mol×K	930.31	Joback Method
dvisc	0.0014835	Pa×s	411.90	Joback Method
dvisc	0.0010154	Pa×s	457.02	Joback Method
dvisc	0.0007441	Pa×s	502.14	Joback Method
dvisc	0.0005739	Pa×s	547.25	Joback Method
dvisc	0.0004605	Pa×s	592.37	Joback Method
dvisc	0.0003812	Pa×s	637.49	Joback Method
dvisc	0.0003235	Pa×s	682.61	Joback Method
hvapt	84.50	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.23342e+01
Coeff. B	-4.27692e+03
Coeff. C	-1.25514e+02
Temperature range (K), min.	480.15
Temperature range (K), max.	734.15

Sources

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
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=C18801008&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
ea: Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume