Anthracene, 9-butyl-

Other names:	9-Butylanthracene
Inchi:	InChI=1S/C18H18/c1-2-3-10-18-16-11-6-4-8-14(16)13-15-9-5-7-12-17(15)18/h4-9,11-13H
InchiKey:	VNCDUSIZHQJFOG-UHFFFAOYSA-N
Formula:	C18H18
SMILES:	CCCCc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	234.34
CAS:	1498-69-7

Physical Properties

Property code	Value	Unit	Source
gf	407.13	kJ/mol	Joback Method
hf	180.88	kJ/mol	Joback Method
hfus	29.68	kJ/mol	Joback Method
hvap	62.54	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.336		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	685.84	K	Joback Method
tc	919.56	K	Joback Method
tf	322.05 ± 0.50	K	NIST Webbook
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.29	J/mol×K	685.84	Joback Method
cpg	550.00	J/mol×K	724.79	Joback Method
cpg	565.55	J/mol×K	763.75	Joback Method
cpg	580.05	J/mol×K	802.70	Joback Method
cpg	593.62	J/mol×K	841.65	Joback Method
cpg	606.39	J/mol×K	880.60	Joback Method
cpg	618.48	J/mol×K	919.56	Joback Method
dvisc	0.0010330	Pa×s	455.54	Joback Method

dvisc	0.0014386	Pa×s	409.48	Joback Method
dvisc	0.0007883	Pa×s	501.60	Joback Method
dvisc	0.0006296	Pa×s	547.66	Joback Method
dvisc	0.0005207	Pa×s	593.72	Joback Method
dvisc	0.0004425	Pa×s	639.78	Joback Method
dvisc	0.0003844	Pa×s	685.84	Joback Method
hsubt	108.10	kJ/mol	303.00	NIST Webbook
hvapt	77.10	kJ/mol	457.00	NIST Webbook
hvapt	83.90	kJ/mol	350.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.53521e+01
Coeff. B	-1.12044e+04
Coeff. C	-4.44180e+01
Temperature range (K), min.	491.15
Temperature range (K), max.	603.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1498697&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
hsubt:	Enthalpy of sublimation at a given temperature
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

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