

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/h4-9,11-13
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	m ³ /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	Paxs	455.54	Joback Method

dvisc	0.0014386	Paxs	409.48	Joback Method
dvisc	0.0007883	Paxs	501.60	Joback Method
dvisc	0.0006296	Paxs	547.66	Joback Method
dvisc	0.0005207	Paxs	593.72	Joback Method
dvisc	0.0004425	Paxs	639.78	Joback Method
dvisc	0.0003844	Paxs	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	$\ln(P_{vp}) = A + B/(T + C)$
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

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=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/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
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

Latest version available from:

<https://www.cheméo.com/cid/73-741-8/Anthracene-9-butyl.pdf>

Generated by Cheméo on 2024-04-24 07:04:03.18776937 +0000 UTC m=+16231492.108346682.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.