

Phenanthrene, 9-butyl-

Other names:	9-Butylphenanthrene
Inchi:	InChI=1S/C18H18/c1-2-3-8-14-13-15-9-4-5-10-17(15)18-12-7-6-11-16(14)18/h4-7,9-13H
InchiKey:	BBQLNZRCZBCVPI-UHFFFAOYSA-N
Formula:	C18H18
SMILES:	CCCCc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]:	234.34
CAS:	10394-57-7

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	409.48	K	Joback Method
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	0.0014386	Paxs	409.48	Joback Method

dvisc	0.0010330	Paxs	455.54	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C10394577&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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