

7-Butylbenz[a]anthracene

Inchi:	InChI=1S/C22H20/c1-2-3-10-20-19-12-7-5-9-17(19)15-22-18-11-6-4-8-16(18)13-14-21(20)
InchiKey:	BIOVWIBRVOHDTA-UHFFFAOYSA-N
Formula:	C22H20
SMILES:	CCCCc1c2ccccc2cc2c1ccc1ccccc12
Mol. weight [g/mol]:	284.39
CAS:	18868-65-0

Physical Properties

Property code	Value	Unit	Source
gf	537.83	kJ/mol	Joback Method
hf	277.92	kJ/mol	Joback Method
hfus	36.67	kJ/mol	Joback Method
hvap	73.75	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	6.489		Crippen Method
mcvol	238.700	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
tb	801.32	K	Joback Method
tc	1043.67	K	Joback Method
tf	499.78	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.57	J/mol×K	801.32	Joback Method
cpg	697.89	J/mol×K	841.71	Joback Method
cpg	713.25	J/mol×K	882.10	Joback Method
cpg	727.85	J/mol×K	922.50	Joback Method
cpg	741.85	J/mol×K	962.89	Joback Method
cpg	755.42	J/mol×K	1003.28	Joback Method
cpg	768.76	J/mol×K	1043.67	Joback Method
dvisc	0.0015546	Pa×s	499.78	Joback Method
dvisc	0.0012104	Pa×s	550.04	Joback Method

dvisc	0.0009827	Pa×s	600.29	Joback Method
dvisc	0.0008240	Pa×s	650.55	Joback Method
dvisc	0.0007086	Pa×s	700.81	Joback Method
dvisc	0.0006218	Pa×s	751.06	Joback Method
dvisc	0.0005546	Pa×s	801.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18868650&Units=SI
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
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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