

Anthracene, 9,10-dibutyl-

Inchi:	InChI=1S/C22H26/c1-3-5-11-17-19-13-7-9-15-21(19)18(12-6-4-2)22-16-10-8-14-20(17)2
InchiKey:	XLTRLRBXMJBVPL-UHFFFAOYSA-N
Formula:	C22H26
SMILES:	CCCCc1c2ccccc2c(CCCC)c2ccccc12
Mol. weight [g/mol]:	290.44
CAS:	1624-34-6

Physical Properties

Property code	Value	Unit	Source
gf	431.18	kJ/mol	Joback Method
hf	86.85	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	6.678		Crippen Method
mcvol	258.160	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
tb	782.34	K	Joback Method
tc	1001.85	K	Joback Method
tf	467.08	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.73	J/mol×K	782.34	Joback Method
cpg	770.45	J/mol×K	818.92	Joback Method
cpg	787.14	J/mol×K	855.51	Joback Method
cpg	802.92	J/mol×K	892.09	Joback Method
cpg	817.88	J/mol×K	928.68	Joback Method
cpg	832.14	J/mol×K	965.26	Joback Method
cpg	845.79	J/mol×K	1001.85	Joback Method
dvisc	0.0011842	Pa×s	467.08	Joback Method
dvisc	0.0008255	Pa×s	519.62	Joback Method

dvisc	0.0006149	Pa×s	572.17	Joback Method
dvisc	0.0004813	Pa×s	624.71	Joback Method
dvisc	0.0003913	Pa×s	677.25	Joback Method
dvisc	0.0003278	Pa×s	729.80	Joback Method
dvisc	0.0002812	Pa×s	782.34	Joback Method

Sources

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=C1624346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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