7,12-Diethylbenz[a]anthracene

Other names: 9,10-Diethyl-1,2-benzanthracene
7,12-Diethylbenz[a]anthracene
Inchi: InChI=1S/C22H20/c1-3-16-19-11-7-8-12-20(19)17(4-2)22-18-10-6-5-9-15(18)13-14-21(1
InchiKey: CIFPUMMYFBMFKK-UHFFFAOYSA-N
Formula: C22H20
SMILES: CCc1c2ccccc2c(CC)c2c1ccc1ccccc12
Mol. weight [g/mol]: 284.40

Physical Properties

Property code	Value	Unit	Source
af	0.6529		Cheméo Relay (1.0)
hf	184.81	kJ/mol	Cheméo Relay (1.0)
hfus	36.28	kJ/mol	Joback Method
hvap	120.07	kJ/mol	Cheméo Relay (1.0)
ie	7.36	eV	Cheméo Relay (1.0)
log10ws	-7.81		Cheméo Relay (1.0)
logp	6.271		Crippen Method
mcvol	238.700	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
tb	731.90	K	Cheméo Relay (1.0)
tc	1010.01	K	Cheméo Relay (1.0)
tf	385.83	K	Cheméo Relay (1.0)
vc	0.900	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.51	J/mol×K	806.30	Joback Method
cpg	696.76	J/mol×K	846.81	Joback Method
cpg	712.09	J/mol×K	887.32	Joback Method
cpg	726.66	J/mol×K	927.84	Joback Method
cpg	740.66	J/mol×K	968.35	Joback Method
cpg	754.24	J/mol×K	1008.86	Joback Method
cpg	767.56	J/mol×K	1049.37	Joback Method

dvisc	0.0014451	Pa×s	512.30	Joback Method
dvisc	0.0011545	Pa×s	561.30	Joback Method
dvisc	0.0009562	Pa×s	610.30	Joback Method
dvisc	0.0008144	Pa×s	659.30	Joback Method
dvisc	0.0007093	Pa×s	708.30	Joback Method
dvisc	0.0006288	Pa×s	757.30	Joback Method
dvisc	0.0005657	Pa×s	806.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16354522&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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