Dibenzo[b,p]chrysene

Inchi: InChI=1S/C26H16/c1-2-9-19-16-25-23-14-13-17-7-3-4-10-20(17)26(23)22-12-6-5-11-21(
InchiKey: IHEBWZXQTKEVFX-UHFFFAOYSA-N
Formula: C26H16
SMILES: c1ccc2cc3c(cc2c1)c1ccccc1c1c2ccccc2ccc31
Mol. weight [g/mol]: 328.41
CAS: 58029-42-8

Physical Properties

Property code	Value	Unit	Source
gf	775.18	kJ/mol	Joback Method
hf	566.03	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-10.49		Crippen Method
logp	7.453		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	935.78	K	Joback Method
tc	1209.93	K	Joback Method
tf	622.78	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.48	J/mol×K	935.78	Joback Method
cpg	838.20	J/mol×K	1164.24	Joback Method
cpg	819.68	J/mol×K	1118.55	Joback Method
cpg	802.30	J/mol×K	1072.85	Joback Method
cpg	785.72	J/mol×K	1027.16	Joback Method
cpg	769.57	J/mol×K	981.47	Joback Method
cpg	858.23	J/mol×K	1209.93	Joback Method
dvisc	0.0017553	Pa×s	935.78	Joback Method
dvisc	0.0018814	Pa×s	883.61	Joback Method

dvisc	0.0020341	Pa×s	831.45	Joback Method
dvisc	0.0022223	Pa×s	779.28	Joback Method
dvisc	0.0024589	Pa×s	727.11	Joback Method
dvisc	0.0027637	Pa×s	674.95	Joback Method
dvisc	0.0031676	Pa×s	622.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58029428&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