Benzo[a]pentacene

Inchi: InChI=1S/C26H16/c1-2-7-19-12-22-15-24-16-26-20(10-9-17-5-3-4-8-25(17)26)13-23(24)
InchiKey: PLKNNIMJRPBOSW-UHFFFAOYSA-N
Formula: C26H16
SMILES: c1ccc2cc3cc4cc5c(ccc6ccccc65)cc4cc3cc2c1
Mol. weight [g/mol]: 328.41
CAS: 239-98-5

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
ie	6.32	eV	NIST Webbook
ie	6.72 ± 0.04	eV	NIST Webbook
ie	6.69	eV	NIST Webbook
ie	6.61 ± 0.02	eV	NIST Webbook
ie	6.72	eV	NIST Webbook
log10ws	-10.49		Crippen Method
logp	7.453		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	624.28		NIST Webbook
rinpol	624.28		NIST Webbook
rinpol	624.03		NIST Webbook
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

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C239985&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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume