Benzo[b]picene

Inchi: InChI=1S/C26H16/c1-2-7-19-16-26-20(15-18(19)6-1)10-12-24-23-11-9-17-5-3-4-8-21(17)
InchiKey: JVVYVDMBJGSYKH-UHFFFAOYSA-N
Formula: C26H16
SMILES: c1ccc2cc3c(ccc4c3ccc3c5ccccc5ccc34)cc2c1
Mol. weight [g/mol]: 328.41
CAS: 217-42-5

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	7.20 ± 0.04	eV	NIST Webbook
ie	7.17 ± 0.02	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	599.06		NIST Webbook
rinpol	599.03		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C217425&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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