Benzo[b]perylene

Inchi: InChI=1S/C24H14/c1-2-9-17-16(6-1)14-22-21-11-4-8-15-7-3-10-19(23(15)21)20-13-5-12-
InchiKey: UXDAAYMFPFYGMU-UHFFFAOYSA-N
Formula: C24H14
SMILES: c1ccc2c(c1)cc1c3cccc4cccc(c5cccc2c51)c43
Mol. weight [g/mol]: 302.37
CAS: 197-70-6

Physical Properties

Property code	Value	Unit	Source
gf	752.58	kJ/mol	Joback Method
hf	561.85	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
ie	6.51	eV	NIST Webbook
ie	6.84	eV	NIST Webbook
ie	6.89	eV	NIST Webbook
ie	6.89	eV	NIST Webbook
ie	6.92 ± 0.04	eV	NIST Webbook
log10ws	-9.91		Crippen Method
logp	6.890		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	556.56		NIST Webbook
rinpol	556.50		NIST Webbook
rinpol	544.51		NIST Webbook
rinpol	586.40		NIST Webbook
tb	882.32	K	Joback Method
tc	1151.38	K	Joback Method
tf	606.52	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	661.66	J/mol×K	882.32	Joback Method
cpg	676.44	J/mol×K	927.16	Joback Method
cpg	691.24	J/mol×K	972.01	Joback Method
cpg	706.42	J/mol×K	1016.85	Joback Method
cpg	722.35	J/mol×K	1061.69	Joback Method
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
dvisc	0.0052883	Pa×s	606.52	Joback Method
dvisc	0.0049439	Pa×s	652.49	Joback Method
dvisc	0.0046630	Pa×s	698.45	Joback Method
dvisc	0.0044300	Pa×s	744.42	Joback Method
dvisc	0.0042338	Pa×s	790.39	Joback Method
dvisc	0.0040664	Pa×s	836.35	Joback Method
dvisc	0.0039222	Pa×s	882.32	Joback Method

Sources

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=C197706&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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