11H-Benzo[a]fluorene

Other names: 1,2-Benzofluorene
Benzo[a]fluorene
Chrysofluorene
Inchi: InChI=1S/C17H12/c1-3-7-14-12(5-1)9-10-16-15-8-4-2-6-13(15)11-17(14)16/h1-10H,11H2
InchiKey: HKMTVMBEALTRRR-UHFFFAOYSA-N
Formula: C17H12
SMILES: c1ccc2c(c1)Cc1c-2ccc2ccccc12
Mol. weight [g/mol]: 216.28
CAS: 238-84-6

Physical Properties

Property code	Value	Unit	Source
gf	487.50	kJ/mol	Joback Method
hf	340.97	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-6.68		Aqueous Solubility Prediction Method
logp	4.411		Crippen Method
mcvol	172.550	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	686.20	K	NIST Webbook
tb	686.00	K	NIST Webbook
tc	937.21	K	Joback Method
tf	462.50 ± 0.50	K	NIST Webbook
tf	462.65	K	Aqueous Solubility Prediction Method
tf	462.80 ± 0.10	K	NIST Webbook
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.86	J/mol×K	678.51	Joback Method

cpg	453.60	J/mol×K	721.63	Joback Method
cpg	467.14	J/mol×K	764.74	Joback Method
cpg	479.68	J/mol×K	807.86	Joback Method
cpg	491.43	J/mol×K	850.98	Joback Method
cpg	502.61	J/mol×K	894.10	Joback Method
cpg	513.42	J/mol×K	937.21	Joback Method
dvisc	0.0009629	Pa×s	678.51	Joback Method
dvisc	0.0016313	Pa×s	474.48	Joback Method
dvisc	0.0014198	Pa×s	515.28	Joback Method
dvisc	0.0012612	Pa×s	556.09	Joback Method
dvisc	0.0019238	Pa×s	433.67	Joback Method
dvisc	0.0010415	Pa×s	637.70	Joback Method
dvisc	0.0011386	Pa×s	596.90	Joback Method
hfust	18.40	kJ/mol	462.80	NIST Webbook
hfust	18.40	kJ/mol	462.80	NIST Webbook
hfust	3.80	kJ/mol	399.90	NIST Webbook
hfust	18.40	kJ/mol	462.80	NIST Webbook
hsubt	105.40	kJ/mol	383.00	NIST Webbook
hvapt	83.70	kJ/mol	398.00	NIST Webbook
sfust	39.70	J/mol×K	462.80	NIST Webbook
sfust	9.50	J/mol×K	399.90	NIST Webbook
sfust	39.76	J/mol×K	462.80	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C238846&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

hfust: Enthalpy of fusion at a given temperature

hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume