

Benzo[a]fluorene

Other names:	1,2-Benzofluorene 11H-Benzo[a]fluorene 1,2-benzfluorene
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:	<chem>c1ccc2c(c1)Cc1c-2ccc2ccccc12</chem>
Mol. weight [g/mol]:	216.28
CAS:	30777-18-5

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	-6.23		Crippen Method
logp	4.411		Crippen Method
mcvol	172.550	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	2167.60		NIST Webbook
rinpol	2228.10		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2167.27		NIST Webbook
rinpol	2153.04		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	364.44		NIST Webbook
rinpol	364.45		NIST Webbook
rinpol	364.86		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	366.50		NIST Webbook
rinpol	366.39		NIST Webbook
rinpol	366.48		NIST Webbook
rinpol	366.64		NIST Webbook

rinpol	366.52		NIST Webbook
rinpol	359.80		NIST Webbook
rinpol	359.80		NIST Webbook
rinpol	366.30		NIST Webbook
rinpol	366.60		NIST Webbook
rinpol	366.56		NIST Webbook
rinpol	366.45		NIST Webbook
rinpol	366.54		NIST Webbook
rinpol	366.44		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	366.30		NIST Webbook
rinpol	366.28		NIST Webbook
rinpol	366.28		NIST Webbook
rinpol	366.54		NIST Webbook
rinpol	366.52		NIST Webbook
rinpol	366.50		NIST Webbook
rinpol	366.70		NIST Webbook
rinpol	366.50		NIST Webbook
rinpol	366.37		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	364.80		NIST Webbook
rinpol	371.80		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	366.92		NIST Webbook
rinpol	367.50		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	362.05		NIST Webbook
rinpol	363.68		NIST Webbook
rinpol	364.92		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	366.74		NIST Webbook
rinpol	366.52		NIST Webbook
rinpol	366.56		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	364.44		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	366.72		NIST Webbook
rinpol	361.25		NIST Webbook
tb	678.51	K	Joback Method
tc	937.21	K	Joback Method
tf	433.67	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.86	J/molxK	678.51	Joback Method
cpg	453.60	J/molxK	721.63	Joback Method
cpg	467.14	J/molxK	764.74	Joback Method
cpg	479.68	J/molxK	807.86	Joback Method
cpg	491.43	J/molxK	850.98	Joback Method
cpg	502.61	J/molxK	894.10	Joback Method
cpg	513.42	J/molxK	937.21	Joback Method
dvisc	0.0019238	Paxs	433.67	Joback Method
dvisc	0.0016313	Paxs	474.48	Joback Method
dvisc	0.0014198	Paxs	515.28	Joback Method
dvisc	0.0012612	Paxs	556.09	Joback Method
dvisc	0.0011386	Paxs	596.90	Joback Method
dvisc	0.0010415	Paxs	637.70	Joback Method
dvisc	0.0009629	Paxs	678.51	Joback Method

Sources

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=C30777185&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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