

11H-Benzo[a]fluoren-11-one

Other names:	11H-Benzo[a]fluorene-11-one 11-benzo[a]fluorenone 1,2-Benzofluorenone
Inchi:	InChI=1S/C17H10O/c18-17-15-8-4-3-7-13(15)14-10-9-11-5-1-2-6-12(11)16(14)17/h1-10H
InchiKey:	RNICURKFVSAHLQ-UHFFFAOYSA-N
Formula:	C17H10O
SMILES:	O=C1c2cccc2-c2ccc3ccccc3c21
Mol. weight [g/mol]:	230.26
CAS:	479-79-8

Physical Properties

Property code	Value	Unit	Source
gf	364.91	kJ/mol	Joback Method
hf	203.27	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.051		Crippen Method
mcvol	174.120	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	386.04		NIST Webbook
rinpol	386.13		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	386.41		NIST Webbook
tb	746.33	K	Joback Method
tc	1015.64	K	Joback Method
tf	501.89	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.25	J/mol×K	746.33	Joback Method
cpg	474.99	J/mol×K	791.21	Joback Method

cpg	487.69	J/mol×K	836.10	Joback Method
cpg	499.53	J/mol×K	880.98	Joback Method
cpg	510.68	J/mol×K	925.87	Joback Method
cpg	521.33	J/mol×K	970.75	Joback Method
cpg	531.63	J/mol×K	1015.64	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=C479798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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