

9-Ethynyl-9-fluorenol

Inchi:	InChI=1S/C15H10O/c1-2-15(16)13-9-5-3-7-11(13)12-8-4-6-10-14(12)15/h1,3-10,16H
InchiKey:	MMZVVJGCZZAWBN-UHFFFAOYSA-N
Formula:	C15H10O
SMILES:	C#CC1(O)c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	206.24
CAS:	13461-74-0

Physical Properties

Property code	Value	Unit	Source
gf	446.69	kJ/mol	Joback Method
hf	337.22	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	2.536		Crippen Method
mcvol	161.100	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	686.66	K	Joback Method
tc	927.61	K	Joback Method
tf	493.36	K	Joback Method
vc	0.612	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.09	J/mol×K	686.66	Joback Method
cpg	418.46	J/mol×K	726.82	Joback Method
cpg	429.29	J/mol×K	766.98	Joback Method
cpg	439.84	J/mol×K	807.14	Joback Method
cpg	450.36	J/mol×K	847.30	Joback Method
cpg	461.10	J/mol×K	887.45	Joback Method
cpg	472.32	J/mol×K	927.61	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=C13461740&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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