

Azuleno[4,5-b]furan-2(3H)-one, 3a,4,6a,7,8,9,9a,9b-octahydro-6-methyl-3,9-bis(methylene)-

Other names:

Epimanthin
Vanillosmine

(3aS,6aR,9aR,9bS)-6-Methyl-3,9-dimethylene-3a,4,6a,7,8,9,9a,9b-octahydroazuleno[4,5-

Inchi:	InChI=1S/C15H18O2/c1-8-4-7-12-10(3)15(16)17-14(12)13-9(2)5-6-11(8)13/h4,11-14H,2-
InchiKey:	BWRZDLYJNURUHS-UHFFFAOYSA-N
Formula:	C15H18O2
SMILES:	C=C1C(=O)OC2C1CC=C(C)C1CCC(=C)C12
Mol. weight [g/mol]:	230.30
CAS:	37936-58-6

Physical Properties

Property code	Value	Unit	Source
gf	119.34	kJ/mol	Joback Method
hf	-234.42	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.017		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2018.00		NIST Webbook
tb	672.46	K	Joback Method
tc	909.11	K	Joback Method
tf	429.74	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.90	J/molxK	672.46	Joback Method
cpg	558.96	J/molxK	711.90	Joback Method
cpg	577.64	J/molxK	751.34	Joback Method
cpg	595.00	J/molxK	790.79	Joback Method
cpg	611.08	J/molxK	830.23	Joback Method

cpg	625.92	J/mol×K	869.67	Joback Method
cpg	639.56	J/mol×K	909.11	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=C37936586&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
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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