

Naphtho(2,3-b)furan-2(3H)-one, decahydro-8a-methyl-3,5-bis(methylene)-, (3aR-(3a«alpha»,4a«alpha»,8a«beta»,9a«alpha»))-

Other names: Eudesma-4(14),11(13)-dien-12-oxic acid, 8-«beta»-hydroxy-, «gamma»-lactone, Isoalantolactone

Inchi:	InChI=1S/C15H20O2/c1-9-5-4-6-15(3)8-13-11(7-12(9)15)10(2)14(16)17-13/h11-13H,1-2,
InchiKey:	CVUANYCQTOGILD-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	C=C1C(=O)OC2CC3(C)CCCC(=C)C3CC12
Mol. weight [g/mol]:	232.32
CAS:	470-17-7

Physical Properties

Property code	Value	Unit	Source
gf	93.52	kJ/mol	Joback Method
hf	-265.49	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	57.03	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.241		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
tb	668.56	K	Joback Method
tc	911.16	K	Joback Method
tf	440.36	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.67	J/molxK	668.56	Joback Method
cpg	580.06	J/molxK	708.99	Joback Method
cpg	600.23	J/molxK	749.43	Joback Method
cpg	619.34	J/molxK	789.86	Joback Method
cpg	637.56	J/molxK	830.29	Joback Method
cpg	655.08	J/molxK	870.73	Joback Method
cpg	672.06	J/molxK	911.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C470177&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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