2(4H)-benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-

Other names: (2,6,6-Trimethyl-2-hydroxycyclohexylidene)acetic acid lactone
4,5,7,7a-Tetrahydro-4,4,7a-trimethyl-2(6H)benzofuranone
4,4,7a-Trimethyl-5,6,7,7a-tetrahydro-4H-Benzofuran-2-one
5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone
(2,6,6-trimethy1-2-hydroxycyclohexylidene)-acetic acid lactone
5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-4H-benzo[b]furan-2-one
Dihydroactinolide
5,6,7,7a-tetrahydro-4,4,7a-trimethylbenzofuran-2(4H)-one

Inchi: InChI=1S/C11H16O2/c1-10(2)5-4-6-11(3)8(10)7-9(12)13-11/h7H,4-6H2,1-3H3

InchiKey: IMKHDCBNRDRUEB-UHFFFAOYSA-N

Formula: C11H16O2

SMILES: CC1(C)CCCC2(C)OC(=O)C=C12

Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
hfus	9.94	kJ/mol	Joback Method
logp	2.438		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
rinpol	1479.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1537.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2332.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2332.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.12	J/mol×K	576.76	Joback Method
cpg	401.95	J/mol×K	617.87	Joback Method

cpg	418.65	J/mol×K	658.98	Joback Method
cpg	434.48	J/mol×K	700.08	Joback Method
cpg	449.74	J/mol×K	741.19	Joback Method
cpg	464.70	J/mol×K	782.30	Joback Method
cpg	479.66	J/mol×K	823.41	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15356748&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices