

Methyl-«beta»-costate

Inchi:	InChI=1S/C16H24O2/c1-11-6-5-8-16(3)9-7-13(10-14(11)16)12(2)15(17)18-4/h13H,2,5-10H
InchiKey:	OWZSHJKGKHTKDS-BBRMVZONSA-N
Formula:	C16H24O2
SMILES:	C=C(C(=O)OC)C1CCC2(C)CCCC(C)=C2C1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
hfus	19.41	kJ/mol	Joback Method
logp	4.022		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
rinpol	1772.00		NIST Webbook
ripol	2304.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.26	J/mol×K	678.25	Joback Method
cpg	629.72	J/mol×K	715.82	Joback Method
cpg	649.10	J/mol×K	753.39	Joback Method
cpg	667.55	J/mol×K	790.96	Joback Method
cpg	685.22	J/mol×K	828.53	Joback Method
cpg	702.26	J/mol×K	866.10	Joback Method
cpg	718.81	J/mol×K	903.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R270012&Units=SI>

Joback Method:

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

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

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