

methyl everninate, acetylated

Inchi:	InChI=1S/C12H14O5/c1-7-5-9(15-3)6-10(17-8(2)13)11(7)12(14)16-4/h5-6H,1-4H3
InchiKey:	SMXWUZTYUCQGAH-UHFFFAOYSA-N
Formula:	C12H14O5
SMILES:	<chem>COC(=O)c1c(C)cc(OC)cc1OC(C)=O</chem>
Mol. weight [g/mol]:	238.24

Physical Properties

Property code	Value	Unit	Source
gf	-439.16	kJ/mol	Joback Method
hf	-710.71	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.716		Crippen Method
mvol	176.930	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	690.58	K	Joback Method
tc	901.91	K	Joback Method
tf	455.53	K	Joback Method
vc	0.665	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.52	J/molxK	690.58	Joback Method
cpg	472.36	J/molxK	725.80	Joback Method
cpg	484.44	J/molxK	761.02	Joback Method
cpg	495.74	J/molxK	796.25	Joback Method
cpg	506.22	J/molxK	831.47	Joback Method
cpg	515.87	J/molxK	866.69	Joback Method
cpg	524.65	J/molxK	901.91	Joback Method
dvisc	0.0005896	Paxs	455.53	Joback Method

dvisc	0.0004037	Paxs	494.70	Joback Method
dvisc	0.0002922	Paxs	533.88	Joback Method
dvisc	0.0002211	Paxs	573.05	Joback Method
dvisc	0.0001734	Paxs	612.23	Joback Method
dvisc	0.0001400	Paxs	651.40	Joback Method
dvisc	0.0001158	Paxs	690.58	Joback Method

Sources

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=R273977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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