

2,3,5,6-(CH₃)₄-C₆H-COOCH₃

Inchi:	InChI=1S/C12H16O2/c1-7-6-8(2)10(4)11(9(7)3)12(13)14-5/h6H,1-5H3
InchiKey:	GMSOGDJHFPQOBM-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	COC(=O)c1c(C)c(C)cc(C)c1C
Mol. weight [g/mol]:	192.25
CAS:	22524-51-2

Physical Properties

Property code	Value	Unit	Source
gf	-109.87	kJ/mol	Joback Method
hf	-345.16	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	56.39	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.707		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	596.85	K	Joback Method
tc	806.77	K	Joback Method
tf	373.66	K	Joback Method
vc	0.624	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.49	J/molxK	596.85	Joback Method
cpg	456.83	J/molxK	771.79	Joback Method
cpg	445.31	J/molxK	736.80	Joback Method
cpg	433.12	J/molxK	701.81	Joback Method
cpg	420.25	J/molxK	666.82	Joback Method
cpg	406.71	J/molxK	631.84	Joback Method
cpg	467.67	J/molxK	806.77	Joback Method
dvisc	0.0001711	Paxs	596.85	Joback Method
dvisc	0.0002053	Paxs	559.65	Joback Method

dvisc	0.0002528	Paxs	522.45	Joback Method
dvisc	0.0003215	Paxs	485.25	Joback Method
dvisc	0.0004254	Paxs	448.06	Joback Method
dvisc	0.0005921	Paxs	410.86	Joback Method
dvisc	0.0008804	Paxs	373.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22524512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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