Methyl tropate

Inchi:	InChI=1S/C10H12O3/c1-13-10(12)9(7-11)8-5-3-2-4-6-8/h2-6,9,11H,7H2,1H3
InchiKey:	OLEWRQVKIUHEJP-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COC(=O)C(CO)c1ccccc1
Mol. weight [g/mol]:	180.20
CAS:	3967-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-227.45	kJ/mol	Joback Method
hf	-415.51	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	0.935		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1418.40		NIST Webbook
rinpol	1429.50		NIST Webbook
tb	622.91	K	Joback Method
tc	825.20	K	Joback Method
tf	346.86	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.77	J/mol×K	622.91	Joback Method
cpg	363.16	J/mol×K	656.63	Joback Method
cpg	373.87	J/mol×K	690.34	Joback Method
cpg	383.91	J/mol×K	724.06	Joback Method
cpg	393.31	J/mol×K	757.77	Joback Method
cpg	402.07	J/mol×K	791.49	Joback Method
cpg	410.23	J/mol×K	825.20	Joback Method

dvisc	0.0050139	Pa×s	346.86	Joback Method
dvisc	0.0015849	Pa×s	392.87	Joback Method
dvisc	0.0006378	Pa×s	438.88	Joback Method
dvisc	0.0003051	Pa×s	484.88	Joback Method
dvisc	0.0001658	Pa×s	530.89	Joback Method
dvisc	0.0000993	Pa×s	576.90	Joback Method
dvisc	0.0000642	Pa×s	622.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3967531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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