Tropic acid, methyl ester

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

Physical Properties

Property code	Value	Unit	Source
af	0.6489		Cheméo Relay (1.0)
hf	-465.71	kJ/mol	Cheméo Relay (1.0)
hfus	19.05	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-1.48		Cheméo Relay (1.0)
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	548.40	K	Cheméo Relay (1.0)
tc	776.87	K	Cheméo Relay (1.0)
tf	325.56	K	Cheméo Relay (1.0)
vc	0.486	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3967531&Units=SI

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

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.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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