ETHYL M-TOLYLACETATE

Other names:	Ethyl m-tolylacetate
	3-Methylphenylacetic acid ethyl ester
	Ethyl m-methylphenylacetate
	m-Tolylacetic acid ethyl ester
	Benzeneacetic acid, 3-methyl-, ethyl ester
	Ethyl 3-tolyacetate
Inchi:	InChI=1S/C11H14O2/c1-3-13-11(12)8-10-6-4-5-9(2)7-10/h4-7H,3,8H2,1-2H3
InchiKey:	RVIWPVAVHHVQIR-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCOC(=O)Cc1cccc(C)c1
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
af	0.5213		Cheméo Relay (1.0)
gf	-89.40	kJ/mol	Joback Method
hf	-369.56	kJ/mol	Cheméo Relay (1.0)
hfus	20.69	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Cheméo Relay (1.0)
ie	8.37	eV	Cheméo Relay (1.0)
log10ws	-2.56		Cheméo Relay (1.0)
logp	2.101		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	510.70	K	NIST Webbook
tc	723.81	K	Cheméo Relay (1.0)
tf	242.26	K	Cheméo Relay (1.0)
vc	0.552	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.15	J/mol×K	559.03	Joback Method
cpg	360.31	J/mol×K	594.08	Joback Method

cpg	373.70	J/mol×K	629.14	Joback Method
cpg	386.36	J/mol×K	664.19	Joback Method
cpg	398.29	J/mol×K	699.24	Joback Method
cpg	409.50	J/mol×K	734.30	Joback Method
cpg	420.01	J/mol×K	769.35	Joback Method
dvisc	0.0017437	Pa×s	324.83	Joback Method
dvisc	0.0009957	Pa×s	363.86	Joback Method
dvisc	0.0006338	Pa×s	402.90	Joback Method
dvisc	0.0004369	Pa×s	441.93	Joback Method
dvisc	0.0003200	Pa×s	480.96	Joback Method
dvisc	0.0002455	Pa×s	520.00	Joback Method
dvisc	0.0001955	Pa×s	559.03	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.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40061550&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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