

ETHYL O-TOLYLACETATE

Other names:	2-Methylphenylacetic acid ethyl ester Ethyl o-methylphenylacetate o-Tolylacetic acid ethyl ester Benzeneacetic acid, 2-methyl-, ethyl ester
Inchi:	InChI=1S/C11H14O2/c1-3-13-11(12)8-10-7-5-4-6-9(10)2/h4-7H,3,8H2,1-2H3
InchiKey:	HTDQOYWJDUMNHX-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCOC(=O)Cc1ccccc1C
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
af	0.5113		Cheméo Relay (1.0)
gf	-89.40	kJ/mol	Joback Method
hf	-365.53	kJ/mol	Cheméo Relay (1.0)
hfus	20.69	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	2.101		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	516.74	K	Cheméo Relay (1.0)
tc	726.88	K	Cheméo Relay (1.0)
tf	262.43	K	Cheméo Relay (1.0)
vc	0.545	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.70	K	0.40	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40291392&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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