ETHYL 3-METHYLBENZOATE

Other names:	Ethyl-3-methylbenzoate
	Ethyl m-toluate
	Benzoic acid, 3-methyl-, ethyl ester
	m-Toluic acid, ethyl ester
	m-Toluylic acid, ethyl ester
Inchi:	InChI=1S/C10H12O2/c1-3-12-10(11)9-6-4-5-8(2)7-9/h4-7H,3H2,1-2H3
InchiKey:	WSJNYOVBJSOQST-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCOC(=O)c1cccc(C)c1
Mol. weight [g/mol]:	164.20

Physical Properties

Property code	Value	Unit	Source
af	0.5218		Cheméo Relay (1.0)
gf	-97.82	kJ/mol	Joback Method
hf	-345.83	kJ/mol	Cheméo Relay (1.0)
hfus	18.10	kJ/mol	Joback Method
hvap	63.68	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.172		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1294.20		NIST Webbook
rinpol	1294.20		NIST Webbook
rinpol	1246.00		NIST Webbook
tb	510.54	K	Cheméo Relay (1.0)
tc	701.70	K	Cheméo Relay (1.0)
tf	247.95	K	Cheméo Relay (1.0)
vc	0.503	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/mol×K	536.15	Joback Method
cpg	313.54	J/mol×K	571.78	Joback Method
cpg	326.10	J/mol×K	607.42	Joback Method
cpg	337.97	J/mol×K	643.05	Joback Method
cpg	349.15	J/mol×K	678.68	Joback Method
cpg	359.66	J/mol×K	714.31	Joback Method
cpg	369.52	J/mol×K	749.95	Joback Method
dvisc	0.0017515	Pa×s	313.56	Joback Method
dvisc	0.0010200	Pa×s	350.66	Joback Method
dvisc	0.0006587	Pa×s	387.76	Joback Method
dvisc	0.0004592	Pa×s	424.86	Joback Method
dvisc	0.0003392	Pa×s	461.95	Joback Method
dvisc	0.0002621	Pa×s	499.05	Joback Method
dvisc	0.0002099	Pa×s	536.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	2.70	NIST Webbook
tbrp	377.20	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120332&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
rinpol:	Non-polar retention indices
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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