

ethyl o-toluate

Other names:	Ethyl o-methylbenzoate
Inchi:	InChI=1S/C10H12O2/c1-3-12-10(11)9-7-5-4-6-8(9)2/h4-7H,3H2,1-2H3
InchiKey:	SOUAXOGPALPTTC-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	164.20
CAS:	87-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-97.82	kJ/mol	Joback Method
hf	-269.47	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.172		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1271.50		NIST Webbook
tb	500.00 ± 2.00	K	NIST Webbook
tb	500.20	K	NIST Webbook
tc	749.95	K	Joback Method
tf	313.56	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/mol×K	536.15	Joback Method
cpg	359.66	J/mol×K	714.31	Joback Method
cpg	349.15	J/mol×K	678.68	Joback Method
cpg	337.97	J/mol×K	643.05	Joback Method
cpg	326.10	J/mol×K	607.42	Joback Method
cpg	313.54	J/mol×K	571.78	Joback Method

cpg	369.52	J/molxK	749.95	Joback Method
dvisc	0.0002099	Paxs	536.15	Joback Method
dvisc	0.0002621	Paxs	499.05	Joback Method
dvisc	0.0003392	Paxs	461.95	Joback Method
dvisc	0.0004592	Paxs	424.86	Joback Method
dvisc	0.0006587	Paxs	387.76	Joback Method
dvisc	0.0010200	Paxs	350.66	Joback Method
dvisc	0.0017515	Paxs	313.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.70	K	97.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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