p-Tolyl isobutyrate

Other names:	Propanoic acid, 2-methyl-, 4-methylphenyl ester
	Isobutyric acid, p-tolyl ester
	p-Cresyl isobutyrate
	p-Methylphenyl isobutyrate
	para-Tolyl isobutyrate
	Paracresyl isobutyrate
	4-Methylphenyl 2-methylpropanoate
Inchi:	InChI=1S/C11H14O2/c1-8(2)11(12)13-10-6-4-9(3)5-7-10/h4-8H,1-3H3
InchiKey:	UPPSFGGDKACIKP-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	Cc1ccc(OC(=O)C(C)C)cc1
Mol. weight [g/mol]:	178.23
CAS:	103-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-91.84	kJ/mol	Joback Method
hf	-295.39	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.556		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1289.10		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1763.00		NIST Webbook
tb	558.59	K	Joback Method
tc	773.47	K	Joback Method
tf	309.83	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.51	J/mol×K	558.59	Joback Method
cpg	361.03	J/mol×K	594.40	Joback Method
cpg	374.76	J/mol×K	630.22	Joback Method
cpg	387.70	J/mol×K	666.03	Joback Method
cpg	399.87	J/mol×K	701.84	Joback Method
cpg	411.28	J/mol×K	737.66	Joback Method
cpg	421.95	J/mol×K	773.47	Joback Method
dvisc	0.0022187	Pa×s	309.83	Joback Method
dvisc	0.0011460	Pa×s	351.29	Joback Method
dvisc	0.0006805	Pa×s	392.75	Joback Method
dvisc	0.0004464	Pa×s	434.21	Joback Method
dvisc	0.0003151	Pa×s	475.67	Joback Method
dvisc	0.0002352	Pa×s	517.13	Joback Method
dvisc	0.0001834	Pa×s	558.59	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103935&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume