para-Tolyl octanoate

Other names:	p-Cresyl caprylate
	n-Octanoic acid p-tolyl ester
	Octanoic acid, 4-methylphenyl ester
	p-Cresyl capryrate
	p-Cresyl octanoate
	p-Tolyl octanoate
	Octanoic acid, p-tolyl ester
	p-Tolyl n-octanoate
	Caprylic acid, p-tolyl ester
Inchi:	InChI=1S/C15H22O2/c1-3-4-5-6-7-8-15(16)17-14-11-9-13(2)10-12-14/h9-12H,3-8H2,1-2
InchiKey:	ALRYNTSLFYRKGF-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCCCC(=O)Oc1ccc(C)cc1
Mol. weight [g/mol]:	234.33
CAS:	59558-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-55.72	kJ/mol	Joback Method
hf	-372.67	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.261		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1755.00		NIST Webbook
ripol	2264.00		NIST Webbook
tb	650.55	K	Joback Method
tc	848.93	K	Joback Method
tf	369.91	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.11	J/mol×K	650.55	Joback Method
cpg	620.31	J/mol×K	815.87	Joback Method
cpg	607.19	J/mol×K	782.80	Joback Method
cpg	593.23	J/mol×K	749.74	Joback Method
cpg	578.41	J/mol×K	716.68	Joback Method
cpg	562.71	J/mol×K	683.61	Joback Method
cpg	632.62	J/mol×K	848.93	Joback Method
dvisc	0.0001350	Pa×s	650.55	Joback Method
dvisc	0.0001728	Pa×s	603.78	Joback Method
dvisc	0.0002306	Pa×s	557.00	Joback Method
dvisc	0.0003243	Pa×s	510.23	Joback Method
dvisc	0.0004887	Pa×s	463.46	Joback Method
dvisc	0.0008075	Pa×s	416.68	Joback Method
dvisc	0.0015149	Pa×s	369.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59558235&Units=SI

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

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