4-(para-Tolyl)-butyric acid

Other names:	4-(p-Tolyl)butyric acid
	Benzenebutanoic acid, 4-methyl-
Inchi:	InChI=1S/C11H14O2/c1-9-5-7-10(8-6-9)3-2-4-11(12)13/h5-8H,2-4H2,1H3,(H,12,13)
InchiKey:	IXWOVMRDYFFXGI-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	Cc1ccc(CCCC(=O)O)cc1
Mol. weight [g/mol]:	178.23
CAS:	4521-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-121.22	kJ/mol	Joback Method
hf	-310.12	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.402		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	628.79	K	Joback Method
tc	827.28	K	Joback Method
tf	328.15 ± 2.00	K	NIST Webbook
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.63	J/mol×K	628.79	Joback Method
cpg	427.19	J/mol×K	794.20	Joback Method
cpg	417.93	J/mol×K	761.12	Joback Method
cpg	408.07	J/mol×K	728.04	Joback Method
cpg	397.58	J/mol×K	694.95	Joback Method
cpg	386.44	J/mol×K	661.87	Joback Method
cpg	435.88	J/mol×K	827.28	Joback Method

dvisc	0.0000758	Pa×s	628.79	Joback Method
dvisc	0.0001127	Pa×s	584.56	Joback Method
dvisc	0.0001788	Pa×s	540.33	Joback Method
dvisc	0.0003078	Pa×s	496.11	Joback Method
dvisc	0.0005896	Pa×s	451.88	Joback Method
dvisc	0.0013004	Pa×s	407.65	Joback Method
dvisc	0.0034768	Pa×s	363.42	Joback Method

Sources

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=C4521226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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