4-(p-Toly)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

Physical Properties

Property code	Value	Unit	Source
af	0.7547		Cheméo Relay (1.0)
hf	-396.37	kJ/mol	Cheméo Relay (1.0)
hfus	23.59	kJ/mol	Joback Method
hvap	98.13	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-2.46		Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	582.86	K	Cheméo Relay (1.0)
tc	782.18	K	Cheméo Relay (1.0)
tf	344.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.63	J/mol×K	628.79	Joback Method
cpg	435.88	J/mol×K	827.28	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
dvisc	0.0003078	Pa×s	496.11	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	0.0034768	Pa×s	363.42	Joback Method
dvisc	0.0005896	Pa×s	451.88	Joback Method
dvisc	0.0013004	Pa×s	407.65	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521226&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point