3-(4-Methylphenyl)propionic acid

Other names:	3-(4-Methylphenyl)propionic acid
	Benzenepropanoic acid, 4-methyl-
	3-(p-Tolyl)propionic acid
Inchi:	InChI=1S/C10H12O2/c1-8-2-4-9(5-3-8)6-7-10(11)12/h2-5H,6-7H2,1H3,(H,11,12)
InchiKey:	LDYGRLNSOKABMM-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	Cc1ccc(CCC(=O)O)cc1
Mol. weight [g/mol]:	164.20

Physical Properties

Property code	Value	Unit	Source
af	0.7165		Cheméo Relay (1.0)
gf	-129.64	kJ/mol	Joback Method
hf	-368.24	kJ/mol	Cheméo Relay (1.0)
hfus	21.00	kJ/mol	Joback Method
hvap	91.57	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	2.012		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	557.05	K	Cheméo Relay (1.0)
tc	767.96	K	Cheméo Relay (1.0)
tf	362.59	K	Cheméo Relay (1.0)
vc	0.486	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.71	J/mol×K	605.91	Joback Method
cpg	337.80	J/mol×K	639.45	Joback Method
cpg	348.25	J/mol×K	672.98	Joback Method
cpg	358.07	J/mol×K	706.52	Joback Method
cpg	367.30	J/mol×K	740.05	Joback Method

cpg	375.96	J/mol×K	773.59	Joback Method
cpg	384.07	J/mol×K	807.12	Joback Method
dvisc	0.0039982	Pa×s	352.15	Joback Method
dvisc	0.0015091	Pa×s	394.44	Joback Method
dvisc	0.0006879	Pa×s	436.74	Joback Method
dvisc	0.0003602	Pa×s	479.03	Joback Method
dvisc	0.0002095	Pa×s	521.32	Joback Method
dvisc	0.0001322	Pa×s	563.62	Joback Method
dvisc	0.0000889	Pa×s	605.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1505506&Units=SI
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):

Legend

af: Acentric Factor
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
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
vc: Critical Volume