2-(4-Methylphenyl)propanoic acid

Other names: Propanoic acid, 2-(4-methylphenyl)
Inchi: InChI=1S/C10H12O2/c1-7-3-5-9(6-4-7)8(2)10(11)12/h3-6,8H,1-2H3,(H,11,12)
InchiKey: KDYOFXPLHVSIHS-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: Cc1ccc(C(C)C(=O)O)cc1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-132.08	kJ/mol	Joback Method
hf	-294.76	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	63.83	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.183		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	605.47	K	Joback Method
tc	810.65	K	Joback Method
tf	337.15	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.18	J/mol×K	605.47	Joback Method
cpg	338.54	J/mol×K	639.67	Joback Method
cpg	349.21	J/mol×K	673.86	Joback Method
cpg	359.23	J/mol×K	708.06	Joback Method
cpg	368.63	J/mol×K	742.25	Joback Method
cpg	377.42	J/mol×K	776.45	Joback Method

cpg	385.64	J/mol×K	810.65	Joback Method
dvisc	0.0058609	Pa×s	337.15	Joback Method
dvisc	0.0019034	Pa×s	381.87	Joback Method
dvisc	0.0007826	Pa×s	426.59	Joback Method
dvisc	0.0003809	Pa×s	471.31	Joback Method
dvisc	0.0002100	Pa×s	516.03	Joback Method
dvisc	0.0001273	Pa×s	560.75	Joback Method
dvisc	0.0000831	Pa×s	605.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R31672&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

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

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