2-(p-Chlorophenyl)-3-methylbutyric acid

Other names:	«alpha»-(p-Chlorophenyl)isovaleric acid
	Benzeneacetic acid, 4-chloro-«alpha»-(1-methylethyl)-
	Butyric acid, 2-(p-chlorophenyl)-3-methyl-
	2-(4-chlorophenyl)-3-methylbutyric acid
Inchi:	InChI=1S/C11H13ClO2/c1-7(2)10(11(13)14)8-3-5-9(12)6-4-8/h3-7,10H,1-2H3,(H,13,14)
InchiKey:	VTJMSIIXXKNIDJ-UHFFFAOYSA-N
Formula:	C11H13ClO2
SMILES:	CC(C)C(C(=O)O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	212.67
CAS:	2012-74-0

Physical Properties

Property code	Value	Unit	Source
gf	-138.03	kJ/mol	Joback Method
hf	-336.42	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	70.05	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.164		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	665.34	K	Joback Method
tc	874.99	K	Joback Method
tf	363.34	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.05	J/mol×K	665.34	Joback Method
cpg	450.08	J/mol×K	840.05	Joback Method
cpg	441.44	J/mol×K	805.10	Joback Method
cpg	432.15	J/mol×K	770.16	Joback Method
cpg	422.18	J/mol×K	735.22	Joback Method

cpg	411.49	J/mol×K	700.28	Joback Method
cpg	458.11	J/mol×K	874.99	Joback Method
dvisc	0.0000561	Pa×s	665.34	Joback Method
dvisc	0.0000867	Pa×s	615.01	Joback Method
dvisc	0.0001448	Pa×s	564.67	Joback Method
dvisc	0.0002675	Pa×s	514.34	Joback Method
dvisc	0.0005645	Pa×s	464.01	Joback Method
dvisc	0.0014286	Pa×s	413.67	Joback Method
dvisc	0.0046762	Pa×s	363.34	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2012740&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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