

3-(4-Chlorophenyl)propionic acid

Inchi:	InChI=1S/C9H9ClO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-2,4-5H,3,6H2,(H,11,12)
InchiKey:	BBSLOKZINKEUCR-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	O=C(O)CCc1ccc(Cl)cc1
Mol. weight [g/mol]:	184.62
CAS:	2019-34-3

Physical Properties

Property code	Value	Unit	Source
gf	-149.99	kJ/mol	Joback Method
hf	-284.58	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.357		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	620.46	K	Joback Method
tc	828.56	K	Joback Method
tf	370.80	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.06	J/molxK	620.46	Joback Method
cpg	344.67	J/molxK	793.88	Joback Method
cpg	337.46	J/molxK	759.19	Joback Method
cpg	329.72	J/molxK	724.51	Joback Method
cpg	321.43	J/molxK	689.83	Joback Method
cpg	312.55	J/molxK	655.14	Joback Method
cpg	351.37	J/molxK	828.56	Joback Method
dvisc	0.0000910	Paxs	620.46	Joback Method
dvisc	0.0001330	Paxs	578.85	Joback Method

dvisc	0.0002062	Paxs	537.24	Joback Method
dvisc	0.0003441	Paxs	495.63	Joback Method
dvisc	0.0006307	Paxs	454.02	Joback Method
dvisc	0.0013065	Paxs	412.41	Joback Method
dvisc	0.0031870	Paxs	370.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2019343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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