

4-Isopropoxy-3-chlorophenylacetic acid

Inchi:	InChI=1S/C11H13ClO3/c1-7(2)15-10-4-3-8(5-9(10)12)6-11(13)14/h3-5,7H,6H2,1-2H3,(H
InchiKey:	IDIYIZMETAUIPJ-UHFFFAOYSA-N
Formula:	C11H13ClO3
SMILES:	CC(C)Oc1ccc(CC(=O)O)cc1Cl
Mol. weight [g/mol]:	228.67

Physical Properties

Property code	Value	Unit	Source
gf	-250.22	kJ/mol	Joback Method
hf	-474.83	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.754		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinqol	1766.00		NIST Webbook
tb	693.18	K	Joback Method
tc	898.11	K	Joback Method
tf	413.09	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.27	J/molxK	693.18	Joback Method
cpg	470.23	J/molxK	863.96	Joback Method
cpg	461.93	J/molxK	829.80	Joback Method
cpg	452.99	J/molxK	795.65	Joback Method
cpg	443.41	J/molxK	761.49	Joback Method
cpg	433.18	J/molxK	727.34	Joback Method
cpg	477.90	J/molxK	898.11	Joback Method
dvisc	0.0000436	Paxs	693.18	Joback Method
dvisc	0.0000633	Paxs	646.50	Joback Method

dvisc	0.0000973	Paxs	599.82	Joback Method
dvisc	0.0001608	Paxs	553.13	Joback Method
dvisc	0.0002918	Paxs	506.45	Joback Method
dvisc	0.0005973	Paxs	459.77	Joback Method
dvisc	0.0014379	Paxs	413.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R31725&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
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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