

5-Chlorovaleric acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C11H12Cl2O2/c12-8-2-1-3-11(14)15-10-6-4-9(13)5-7-10/h4-7H,1-3,8H2
InchiKey:	ZSYKPxRQYIMAOb-UHFFFAOYSA-N
Formula:	C11H12Cl2O2
SMILES:	O=C(CCCCCl)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	247.12

Physical Properties

Property code	Value	Unit	Source
gf	-113.26	kJ/mol	Joback Method
hf	-321.59	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.655		Crippen Method
mvol	174.010	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1780.00		NIST Webbook
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tb	633.89	K	Joback Method
tc	851.92	K	Joback Method
tf	384.67	K	Joback Method
vc	0.665	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.03	J/mol×K	633.89	Joback Method
cpg	452.30	J/mol×K	815.59	Joback Method
cpg	442.95	J/mol×K	779.25	Joback Method
cpg	432.86	J/mol×K	742.91	Joback Method
cpg	422.03	J/mol×K	706.57	Joback Method
cpg	410.43	J/mol×K	670.23	Joback Method
cpg	460.95	J/mol×K	851.92	Joback Method
dvisc	0.0001806	Paxs	633.89	Joback Method

dvisc	0.0002263	Paxs	592.35	Joback Method
dvisc	0.0002934	Paxs	550.82	Joback Method
dvisc	0.0003969	Paxs	509.28	Joback Method
dvisc	0.0005664	Paxs	467.74	Joback Method
dvisc	0.0008662	Paxs	426.21	Joback Method
dvisc	0.0014521	Paxs	384.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307975&Units=SI

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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