5-Chlorovaleric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H11Cl3O2/c12-6-2-1-3-11(15)16-8-4-5-9(13)10(14)7-8/h4-5,7H,1-3,6H2
InchiKey: BYNHRZMXLGSQAV-UHFFFAOYSA-N
Formula: C11H11Cl3O2
SMILES: O=C(CCCCCl)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 281.56

Physical Properties

Property code	Value	Unit	Source
gf	-134.82	kJ/mol	Joback Method
hf	-348.80	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.308		Crippen Method
mcvol	186.250	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	676.30	K	Joback Method
tc	898.44	K	Joback Method
tf	427.11	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.38	J/mol×K	676.30	Joback Method
cpg	431.66	J/mol×K	713.32	Joback Method
cpg	442.18	J/mol×K	750.35	Joback Method
cpg	451.95	J/mol×K	787.37	Joback Method
cpg	461.00	J/mol×K	824.40	Joback Method
cpg	469.33	J/mol×K	861.42	Joback Method
cpg	476.98	J/mol×K	898.44	Joback Method
dvisc	0.0010595	Pa×s	427.11	Joback Method

dvisc	0.0006769	Pa×s	468.64	Joback Method
dvisc	0.0004652	Pa×s	510.17	Joback Method
dvisc	0.0003383	Pa×s	551.71	Joback Method
dvisc	0.0002572	Pa×s	593.24	Joback Method
dvisc	0.0002027	Pa×s	634.77	Joback Method
dvisc	0.0001645	Pa×s	676.30	Joback Method

Sources

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=U307979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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