Acetic acid, (4-chlorophenoxy)-, butyl ester

Inchi: InChI=1S/C12H15ClO3/c1-2-3-8-15-12(14)9-16-11-6-4-10(13)5-7-11/h4-7H,2-3,8-9H2,1H
InchiKey: GZKDUBJVOZXJOU-UHFFFAOYSA-N
Formula: C12H15ClO3
SMILES: CCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 242.70

Physical Properties

Property code	Value	Unit	Source
gf	-197.91	kJ/mol	Joback Method
hf	-458.71	kJ/mol	Joback Method
hfus	28.66	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.062		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	641.76	K	Joback Method
tc	850.40	K	Joback Method
tf	388.25	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.54	J/mol×K	641.76	Joback Method
cpg	460.30	J/mol×K	676.53	Joback Method
cpg	473.27	J/mol×K	711.31	Joback Method
cpg	485.45	J/mol×K	746.08	Joback Method
cpg	496.85	J/mol×K	780.85	Joback Method
cpg	507.48	J/mol×K	815.63	Joback Method
cpg	517.34	J/mol×K	850.40	Joback Method
dvisc	0.0011397	Pa×s	388.25	Joback Method

dvisc	0.0006730	Pa×s	430.50	Joback Method
dvisc	0.0004366	Pa×s	472.75	Joback Method
dvisc	0.0003041	Pa×s	515.00	Joback Method
dvisc	0.0002237	Pa×s	557.26	Joback Method
dvisc	0.0001719	Pa×s	599.51	Joback Method
dvisc	0.0001367	Pa×s	641.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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