

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

Inchi:	InChI=1S/C12H15ClO3/c1-9(2)7-16-12(14)8-15-11-5-3-10(13)4-6-11/h3-6,9H,7-8H2,1-2H
InchiKey:	KPZQJZLKVMNLLD-UHFFFAOYSA-N
Formula:	C12H15ClO3
SMILES:	CC(C)COC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	242.70

Physical Properties

Property code	Value	Unit	Source
gf	-200.35	kJ/mol	Joback Method
hf	-463.99	kJ/mol	Joback Method
hfus	25.14	kJ/mol	Joback Method
hvap	60.81	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.918		Crippen Method
mvol	181.730	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
tb	641.32	K	Joback Method
tc	854.00	K	Joback Method
tf	373.25	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.02	J/molxK	641.32	Joback Method
cpg	509.09	J/molxK	818.55	Joback Method
cpg	498.32	J/molxK	783.10	Joback Method
cpg	486.73	J/molxK	747.66	Joback Method
cpg	474.32	J/molxK	712.21	Joback Method
cpg	461.09	J/molxK	676.77	Joback Method
cpg	519.05	J/molxK	854.00	Joback Method
dvisc	0.0001271	Paxs	641.32	Joback Method

dvisc	0.0001629	Paxs	596.64	Joback Method
dvisc	0.0002172	Paxs	551.96	Joback Method
dvisc	0.0003047	Paxs	507.28	Joback Method
dvisc	0.0004564	Paxs	462.61	Joback Method
dvisc	0.0007453	Paxs	417.93	Joback Method
dvisc	0.0013687	Paxs	373.25	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=U415095&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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