

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

Inchi:	InChI=1S/C17H25ClO3/c1-2-3-4-5-6-7-8-13-20-17(19)14-21-16-11-9-15(18)10-12-16/h9
InchiKey:	HMSKSBRSVCVSHCI-UHFFFAOYSA-N
Formula:	C17H25ClO3
SMILES:	CCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	312.83

Physical Properties

Property code	Value	Unit	Source
gf	-155.81	kJ/mol	Joback Method
hf	-561.91	kJ/mol	Joback Method
hfus	41.61	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.013		Crippen Method
mvol	252.180	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook
tb	756.16	K	Joback Method
tc	953.73	K	Joback Method
tf	444.60	K	Joback Method
vc	0.971	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.67	J/molxK	756.16	Joback Method
cpg	783.65	J/molxK	920.80	Joback Method
cpg	771.54	J/molxK	887.87	Joback Method
cpg	758.50	J/molxK	854.95	Joback Method
cpg	744.52	J/molxK	822.02	Joback Method
cpg	729.58	J/molxK	789.09	Joback Method
cpg	794.85	J/molxK	953.73	Joback Method
dvisc	0.0000743	Paxs	756.16	Joback Method

dvisc	0.0000953	Paxs	704.23	Joback Method
dvisc	0.0001272	Paxs	652.31	Joback Method
dvisc	0.0001785	Paxs	600.38	Joback Method
dvisc	0.0002671	Paxs	548.45	Joback Method
dvisc	0.0004348	Paxs	496.53	Joback Method
dvisc	0.0007931	Paxs	444.60	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=U415102&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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