

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

Inchi: InChI=1S/C14H19ClO3/c1-2-3-4-5-10-17-14(16)11-18-13-8-6-12(15)7-9-13/h6-9H,2-5,10H
InchiKey: MDWBAMOKXLBIRQ-UHFFFAOYSA-N
Formula: C14H19ClO3
SMILES: CCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 270.75

Physical Properties

Property code	Value	Unit	Source
gf	-181.07	kJ/mol	Joback Method
hf	-499.99	kJ/mol	Joback Method
hfus	33.84	kJ/mol	Joback Method
hvap	65.65	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.842		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	2485.00		NIST Webbook
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tb	687.52	K	Joback Method
tc	890.48	K	Joback Method
tf	410.79	K	Joback Method
vc	0.802	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.60	J/molxK	687.52	Joback Method
cpg	564.42	J/molxK	721.35	Joback Method
cpg	578.37	J/molxK	755.17	Joback Method
cpg	591.46	J/molxK	789.00	Joback Method
cpg	603.70	J/molxK	822.83	Joback Method
cpg	615.10	J/molxK	856.66	Joback Method
cpg	625.67	J/molxK	890.48	Joback Method
dvisc	0.0010061	Paxs	410.79	Joback Method

dvisc	0.0005756	Paxs	456.91	Joback Method
dvisc	0.0003648	Paxs	503.03	Joback Method
dvisc	0.0002496	Paxs	549.15	Joback Method
dvisc	0.0001812	Paxs	595.28	Joback Method
dvisc	0.0001377	Paxs	641.40	Joback Method
dvisc	0.0001085	Paxs	687.52	Joback Method

Sources

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=U415099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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