

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

Inchi:	InChI=1S/C16H23ClO3/c1-2-3-4-5-6-7-12-19-16(18)13-20-15-10-8-14(17)9-11-15/h8-11H
InchiKey:	BFWWNTXCTLPQTR-UHFFFAOYSA-N
Formula:	C16H23ClO3
SMILES:	CCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	298.81

Physical Properties

Property code	Value	Unit	Source
gf	-164.23	kJ/mol	Joback Method
hf	-541.27	kJ/mol	Joback Method
hfus	39.02	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.623		Crippen Method
mvol	238.090	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	733.28	K	Joback Method
tc	932.17	K	Joback Method
tf	433.33	K	Joback Method
vc	0.914	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.83	J/molxK	733.28	Joback Method
cpg	673.43	J/molxK	766.43	Joback Method
cpg	688.09	J/molxK	799.58	Joback Method
cpg	701.82	J/molxK	832.73	Joback Method
cpg	714.64	J/molxK	865.88	Joback Method
cpg	726.56	J/molxK	899.02	Joback Method
cpg	737.60	J/molxK	932.17	Joback Method
dvisc	0.0008637	Paxs	433.33	Joback Method

dvisc	0.0004800	Paxs	483.32	Joback Method
dvisc	0.0002978	Paxs	533.31	Joback Method
dvisc	0.0002006	Paxs	583.30	Joback Method
dvisc	0.0001438	Paxs	633.30	Joback Method
dvisc	0.0001082	Paxs	683.29	Joback Method
dvisc	0.0000846	Paxs	733.28	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=U415101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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