

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

Inchi:	InChI=1S/C18H27ClO3/c1-2-3-4-5-6-7-8-9-14-21-18(20)15-22-17-12-10-16(19)11-13-17
InchiKey:	IYEKAGHJDDMHEC-UHFFFAOYSA-N
Formula:	C18H27ClO3
SMILES:	CCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	326.86

Physical Properties

Property code	Value	Unit	Source
gf	-147.39	kJ/mol	Joback Method
hf	-582.55	kJ/mol	Joback Method
hfus	44.20	kJ/mol	Joback Method
hvap	74.55	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.403		Crippen Method
mvol	266.270	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2899.00		NIST Webbook
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tb	779.04	K	Joback Method
tc	975.83	K	Joback Method
tf	455.87	K	Joback Method
vc	1.026	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.54	J/molxK	779.04	Joback Method
cpg	786.73	J/molxK	811.84	Joback Method
cpg	801.92	J/molxK	844.64	Joback Method
cpg	816.11	J/molxK	877.43	Joback Method
cpg	829.32	J/molxK	910.23	Joback Method
cpg	841.59	J/molxK	943.03	Joback Method
cpg	852.92	J/molxK	975.83	Joback Method
dvisc	0.0007244	Paxs	455.87	Joback Method

dvisc	0.0003920	Paxs	509.73	Joback Method
dvisc	0.0002385	Paxs	563.59	Joback Method
dvisc	0.0001583	Paxs	617.45	Joback Method
dvisc	0.0001122	Paxs	671.32	Joback Method
dvisc	0.0000837	Paxs	725.18	Joback Method
dvisc	0.0000650	Paxs	779.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415103&Units=SI
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

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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