

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

Inchi:	InChI=1S/C15H21ClO3/c1-2-3-4-5-6-11-18-15(17)12-19-14-9-7-13(16)8-10-14/h7-10H,2
InchiKey:	OUXFIMPFXKORKT-UHFFFAOYSA-N
Formula:	C15H21ClO3
SMILES:	CCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	284.78

Physical Properties

Property code	Value	Unit	Source
gf	-172.65	kJ/mol	Joback Method
hf	-520.63	kJ/mol	Joback Method
hfus	36.43	kJ/mol	Joback Method
hvap	67.87	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.232		Crippen Method
mvol	224.000	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	710.40	K	Joback Method
tc	911.11	K	Joback Method
tf	422.06	K	Joback Method
vc	0.859	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.11	J/molxK	710.40	Joback Method
cpg	670.37	J/molxK	877.66	Joback Method
cpg	658.68	J/molxK	844.20	Joback Method
cpg	646.13	J/molxK	810.75	Joback Method
cpg	632.69	J/molxK	777.30	Joback Method
cpg	618.35	J/molxK	743.85	Joback Method
cpg	681.20	J/molxK	911.11	Joback Method
dvisc	0.0000960	Paxs	710.40	Joback Method

dvisc	0.0001223	Paxs	662.34	Joback Method
dvisc	0.0001617	Paxs	614.29	Joback Method
dvisc	0.0002243	Paxs	566.23	Joback Method
dvisc	0.0003305	Paxs	518.17	Joback Method
dvisc	0.0005272	Paxs	470.12	Joback Method
dvisc	0.0009352	Paxs	422.06	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=U415100&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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