

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

Inchi:	InChI=1S/C24H39ClO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-27-24(26)21-28-23-18
InchiKey:	JWNNWWGRPGWOPQ-UHFFFAOYSA-N
Formula:	C24H39ClO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	411.02

Physical Properties

Property code	Value	Unit	Source
gf	-96.87	kJ/mol	Joback Method
hf	-706.39	kJ/mol	Joback Method
hfus	59.74	kJ/mol	Joback Method
hvap	87.91	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.743		Crippen Method
mvol	350.810	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2252.00		NIST Webbook
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tb	916.32	K	Joback Method
tc	1122.53	K	Joback Method
tf	523.49	K	Joback Method
vc	1.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.40	J/molxK	916.32	Joback Method
cpg	1147.10	J/molxK	950.69	Joback Method
cpg	1163.50	J/molxK	985.06	Joback Method
cpg	1178.63	J/molxK	1019.42	Joback Method
cpg	1192.54	J/molxK	1053.79	Joback Method
cpg	1205.25	J/molxK	1088.16	Joback Method
cpg	1216.82	J/molxK	1122.53	Joback Method
dvisc	0.0003834	Paxs	523.49	Joback Method

dvisc	0.0001937	Paxs	588.96	Joback Method
dvisc	0.0001122	Paxs	654.43	Joback Method
dvisc	0.0000718	Paxs	719.90	Joback Method
dvisc	0.0000495	Paxs	785.38	Joback Method
dvisc	0.0000361	Paxs	850.85	Joback Method
dvisc	0.0000276	Paxs	916.32	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=U415109&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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