

Acetic acid, (4-chloro-2-methylphenoxy)-, octadecyl ester

Inchi:	InChI=1S/C27H45ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-30-27(29)23-3
InchiKey:	OWCNDGYJAPUIET-UHFFFAOYSA-N
Formula:	C27H45ClO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)COc1ccc(Cl)cc1C
Mol. weight [g/mol]:	453.10

Physical Properties

Property code	Value	Unit	Source
gf	-81.24	kJ/mol	Joback Method
hf	-779.78	kJ/mol	Joback Method
hfus	67.12	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	8.832		Crippen Method
mvol	393.080	ml/mol	McGowan Method
pc	808.45	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	989.94	K	Joback Method
tc	1213.84	K	Joback Method
tf	569.82	K	Joback Method
vc	1.530	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.80	J/molxK	989.94	Joback Method
cpg	1394.15	J/molxK	1176.52	Joback Method
cpg	1381.69	J/molxK	1139.20	Joback Method
cpg	1367.77	J/molxK	1101.89	Joback Method
cpg	1352.36	J/molxK	1064.57	Joback Method
cpg	1335.38	J/molxK	1027.26	Joback Method
cpg	1405.23	J/molxK	1213.84	Joback Method
dvisc	0.0000179	Paxs	989.94	Joback Method

dvisc	0.0000233	Paxs	919.92	Joback Method
dvisc	0.0000317	Paxs	849.90	Joback Method
dvisc	0.0000457	Paxs	779.88	Joback Method
dvisc	0.0000706	Paxs	709.86	Joback Method
dvisc	0.0001201	Paxs	639.84	Joback Method
dvisc	0.0002328	Paxs	569.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	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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