Phenylacetic acid, 4-chloro-, pentadecyl ester

Inchi: InChI=1S/C23H37ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-26-23(25)20-21-15-17-22(
InchiKey: RIBKIEWMPDYZQU-UHFFFAOYSA-N
Formula: C23H37ClO2
SMILES: CCCCCCCCCCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 380.99

Physical Properties

Property code	Value	Unit	Source
gf	-0.29	kJ/mol	Joback Method
hf	-553.53	kJ/mol	Joback Method
hfus	55.96	kJ/mol	Joback Method
hvap	83.27	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.517		Crippen Method
mcvol	330.850	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	871.02	K	Joback Method
tc	1070.81	K	Joback Method
tf	489.99	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.11	J/mol×K	871.02	Joback Method
cpg	1054.99	J/mol×K	904.32	Joback Method
cpg	1071.72	J/mol×K	937.62	Joback Method
cpg	1087.36	J/mol×K	970.92	Joback Method
cpg	1101.93	J/mol×K	1004.22	Joback Method
cpg	1115.50	J/mol×K	1037.51	Joback Method
cpg	1128.11	J/mol×K	1070.81	Joback Method
dvisc	0.0006243	Pa×s	489.99	Joback Method

dvisc	0.0003094	Pa×s	553.50	Joback Method
dvisc	0.0001772	Pa×s	617.00	Joback Method
dvisc	0.0001126	Pa×s	680.50	Joback Method
dvisc	0.0000773	Pa×s	744.01	Joback Method
dvisc	0.0000563	Pa×s	807.51	Joback Method
dvisc	0.0000430	Pa×s	871.02	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=U406218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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