Phenylacetic acid, 4-chloro-, hexadecyl ester

Inchi: InChI=1S/C24H39ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-27-24(26)21-22-16-18-
InchiKey: GADWPBWMJAECSO-UHFFFAOYSA-N
Formula: C24H39ClO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 395.02

Physical Properties

Property code	Value	Unit	Source
gf	8.13	kJ/mol	Joback Method
hf	-574.17	kJ/mol	Joback Method
hfus	58.55	kJ/mol	Joback Method
hvap	85.50	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.907		Crippen Method
mcvol	344.940	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinpol	2991.00		NIST Webbook
rinpol	2991.00		NIST Webbook
tb	893.90	K	Joback Method
tc	1096.46	K	Joback Method
tf	501.26	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.56	J/mol×K	893.90	Joback Method
cpg	1116.74	J/mol×K	927.66	Joback Method
cpg	1133.72	J/mol×K	961.42	Joback Method
cpg	1149.56	J/mol×K	995.18	Joback Method
cpg	1164.31	J/mol×K	1028.94	Joback Method
cpg	1178.02	J/mol×K	1062.70	Joback Method
cpg	1190.73	J/mol×K	1096.46	Joback Method
dvisc	0.0005578	Pa×s	501.26	Joback Method

dvisc	0.0002736	Pa×s	566.70	Joback Method
dvisc	0.0001555	Pa×s	632.14	Joback Method
dvisc	0.0000983	Pa×s	697.58	Joback Method
dvisc	0.0000672	Pa×s	763.02	Joback Method
dvisc	0.0000488	Pa×s	828.46	Joback Method
dvisc	0.0000371	Pa×s	893.90	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=U406219&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