Phenylacetic acid, 4-chloro-, tridecyl ester

Inchi: InChI=1S/C21H33ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-21(23)18-19-13-15-20(22)16-
InchiKey: LECJSGBIFXEKSF-UHFFFAOYSA-N
Formula: C21H33ClO2
SMILES: CCCCCCCCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 352.94

Physical Properties

Property code	Value	Unit	Source
gf	-17.13	kJ/mol	Joback Method
hf	-512.25	kJ/mol	Joback Method
hfus	50.78	kJ/mol	Joback Method
hvap	78.82	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.737		Crippen Method
mcvol	302.670	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	2682.00		NIST Webbook
rinpol	2682.00		NIST Webbook
tb	825.26	K	Joback Method
tc	1021.88	K	Joback Method
tf	467.45	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.32	J/mol×K	825.26	Joback Method
cpg	992.75	J/mol×K	989.11	Joback Method
cpg	979.45	J/mol×K	956.34	Joback Method
cpg	965.19	J/mol×K	923.57	Joback Method
cpg	949.95	J/mol×K	890.80	Joback Method
cpg	933.67	J/mol×K	858.03	Joback Method
cpg	1005.13	J/mol×K	1021.88	Joback Method
dvisc	0.0000571	Pa×s	825.26	Joback Method

dvisc	0.0000744	Pa×s	765.62	Joback Method
dvisc	0.0001014	Pa×s	705.99	Joback Method
dvisc	0.0001464	Pa×s	646.36	Joback Method
dvisc	0.0002278	Pa×s	586.72	Joback Method
dvisc	0.0003916	Pa×s	527.09	Joback Method
dvisc	0.0007730	Pa×s	467.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406216&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