Phenylacetic acid, 4-chloro-, dodecyl ester

Inchi: InChI=1S/C20H31ClO2/c1-2-3-4-5-6-7-8-9-10-11-16-23-20(22)17-18-12-14-19(21)15-13-

InchiKey: SVPRXBKABDSHJT-UHFFFAOYSA-N

Formula: C20H31ClO2

SMILES: CCCCCCCCCCCCOC(=O)Cc1ccc(Cl)cc1

Mol. weight [g/mol]: 338.91

Physical Properties

Property code	Value	Unit	Source
gf	-25.55	kJ/mol	Joback Method
hf	-491.61	kJ/mol	Joback Method
hfus	48.19	kJ/mol	Joback Method
hvap	76.59	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.347		Crippen Method
mcvol	288.580	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	802.38	K	Joback Method
tc	998.48	K	Joback Method
tf	456.18	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.11	J/mol×K	802.38	Joback Method
cpg	874.21	J/mol×K	835.06	Joback Method
cpg	890.26	J/mol×K	867.75	Joback Method
cpg	905.32	J/mol×K	900.43	Joback Method
cpg	919.41	J/mol×K	933.11	Joback Method
cpg	932.56	J/mol×K	965.79	Joback Method
cpg	944.82	J/mol×K	998.48	Joback Method
dvisc	0.0008547	Pa×s	456.18	Joback Method

dvisc	0.0004381	Pa×s	513.88	Joback Method
dvisc	0.0002570	Pa×s	571.58	Joback Method
dvisc	0.0001662	Pa×s	629.28	Joback Method
dvisc	0.0001157	Pa×s	686.98	Joback Method
dvisc	0.0000852	Pa×s	744.68	Joback Method
dvisc	0.0000655	Pa×s	802.38	Joback Method

Sources

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=U406215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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