4-(4-Chloro-2-methylphenoxy)butyric acid, pentadecyl ester

Inchi: InChI=1S/C26H43ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-30-26(28)17-16-21-29-25
InchiKey: UVLNCXJMFBDJKT-UHFFFAOYSA-N
Formula: C26H43ClO3
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]: 439.07

Physical Properties

Property code	Value	Unit	Source
gf	-89.66	kJ/mol	Joback Method
hf	-759.14	kJ/mol	Joback Method
hfus	64.53	kJ/mol	Joback Method
hvap	93.02	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	8.442		Crippen Method
mcvol	378.990	ml/mol	McGowan Method
pc	854.46	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	967.06	K	Joback Method
tc	1184.35	K	Joback Method
tf	558.55	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.73	J/mol×K	967.06	Joback Method
cpg	1271.96	J/mol×K	1003.28	Joback Method
cpg	1288.69	J/mol×K	1039.49	Joback Method
cpg	1303.97	J/mol×K	1075.71	Joback Method
cpg	1317.83	J/mol×K	1111.92	Joback Method
cpg	1330.34	J/mol×K	1148.14	Joback Method
cpg	1341.52	J/mol×K	1184.35	Joback Method
dvisc	0.0002627	Pa×s	558.55	Joback Method

dvisc	0.0001369	Pa×s	626.63	Joback Method
dvisc	0.0000810	Pa×s	694.72	Joback Method
dvisc	0.0000527	Pa×s	762.80	Joback Method
dvisc	0.0000368	Pa×s	830.89	Joback Method
dvisc	0.0000271	Pa×s	898.97	Joback Method
dvisc	0.0000208	Pa×s	967.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415091&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

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