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

Inchi: InChI=1S/C28H47ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-32-28(30)19-18-23

InchiKey: CDWBUDGEQQEMLQ-UHFFFAOYSA-N

Formula: C28H47ClO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCOc1ccc(Cl)cc1C

Mol. weight [g/mol]: 467.12

Physical Properties

Property code	Value	Unit	Source
gf	-72.82	kJ/mol	Joback Method
hf	-800.42	kJ/mol	Joback Method
hfus	69.71	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-9.99		Crippen Method
logp	9.222		Crippen Method
mcvol	407.170	ml/mol	McGowan Method
pc	766.06	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	1012.82	K	Joback Method
tc	1244.48	K	Joback Method
tf	581.09	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.25	J/mol×K	1012.82	Joback Method
cpg	1458.39	J/mol×K	1205.87	Joback Method
cpg	1445.98	J/mol×K	1167.26	Joback Method
cpg	1432.03	J/mol×K	1128.65	Joback Method
cpg	1416.46	J/mol×K	1090.04	Joback Method
cpg	1399.23	J/mol×K	1051.43	Joback Method
cpg	1469.32	J/mol×K	1244.48	Joback Method
dvisc	0.0000153	Pa×s	1012.82	Joback Method

dvisc	0.0000200	Pa×s	940.86	Joback Method
dvisc	0.0000273	Pa×s	868.91	Joback Method
dvisc	0.0000395	Pa×s	796.95	Joback Method
dvisc	0.0000614	Pa×s	725.00	Joback Method
dvisc	0.0001051	Pa×s	653.04	Joback Method
dvisc	0.0002057	Pa×s	581.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415093&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