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

Inchi: InChI=1S/C20H31ClO3/c1-3-4-5-6-7-8-9-14-24-20(22)11-10-15-23-19-13-12-18(21)16-17

InchiKey: LLQUOUYJTSRTAG-UHFFFAOYSA-N

Formula: C20H31ClO3

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

Mol. weight [g/mol]: 354.91

Physical Properties

Property code	Value	Unit	Source
gf	-140.18	kJ/mol	Joback Method
hf	-635.30	kJ/mol	Joback Method
hfus	48.99	kJ/mol	Joback Method
hvap	79.66	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.101		Crippen Method
mcvol	294.450	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	3106.00		NIST Webbook
rinpol	3106.00		NIST Webbook
tb	829.78	K	Joback Method
tc	1027.67	K	Joback Method
tf	490.93	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.57	J/mol×K	829.78	Joback Method
cpg	903.18	J/mol×K	862.76	Joback Method
cpg	918.70	J/mol×K	895.74	Joback Method
cpg	933.15	J/mol×K	928.73	Joback Method
cpg	946.56	J/mol×K	961.71	Joback Method
cpg	958.93	J/mol×K	994.69	Joback Method
cpg	970.30	J/mol×K	1027.67	Joback Method
dvisc	0.0005066	Pa×s	490.93	Joback Method

dvisc	0.0002821	Pa×s	547.40	Joback Method
dvisc	0.0001753	Pa×s	603.88	Joback Method
dvisc	0.0001181	Pa×s	660.36	Joback Method
dvisc	0.0000847	Pa×s	716.83	Joback Method
dvisc	0.0000638	Pa×s	773.31	Joback Method
dvisc	0.0000499	Pa×s	829.78	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=U415085&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