

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

Inchi:	InChI=1S/C23H37ClO3/c1-3-4-5-6-7-8-9-10-11-12-17-27-23(25)14-13-18-26-22-16-15-2
InchiKey:	XNJZMRSIYQLCAX-UHFFFAOYSA-N
Formula:	C23H37ClO3
SMILES:	CCCCCCCCCCCCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]:	396.99

Physical Properties

Property code	Value	Unit	Source
gf	-114.92	kJ/mol	Joback Method
hf	-697.22	kJ/mol	Joback Method
hfus	56.76	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.272		Crippen Method
mcvol	336.720	ml/mol	McGowan Method
pc	1018.78	kPa	Joback Method
rinpol	3424.00		NIST Webbook
tb	898.42	K	Joback Method
tc	1102.09	K	Joback Method
tf	524.74	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.40	J/molxK	898.42	Joback Method
cpg	1141.90	J/molxK	1068.14	Joback Method
cpg	1129.39	J/molxK	1034.20	Joback Method
cpg	1115.71	J/molxK	1000.25	Joback Method
cpg	1100.84	J/molxK	966.31	Joback Method
cpg	1084.75	J/molxK	932.36	Joback Method
cpg	1153.27	J/molxK	1102.09	Joback Method
dvisc	0.0000326	Paxs	898.42	Joback Method
dvisc	0.0000420	Paxs	836.14	Joback Method

dvisc	0.0000564	Paxs	773.86	Joback Method
dvisc	0.0000798	Paxs	711.58	Joback Method
dvisc	0.0001207	Paxs	649.30	Joback Method
dvisc	0.0001993	Paxs	587.02	Joback Method
dvisc	0.0003707	Paxs	524.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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