

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

Inchi:	InChI=1S/C15H21ClO3/c1-3-4-9-19-15(17)6-5-10-18-14-8-7-13(16)11-12(14)2/h7-8,11H,
InchiKey:	KOXLMFVJUQQBIY-UHFFFAOYSA-N
Formula:	C15H21ClO3
SMILES:	CCCCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]:	284.78

Physical Properties

Property code	Value	Unit	Source
gf	-182.28	kJ/mol	Joback Method
hf	-532.10	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.151		Crippen Method
mvol	224.000	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2485.00		NIST Webbook
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tb	715.38	K	Joback Method
tc	916.91	K	Joback Method
tf	434.58	K	Joback Method
vc	0.859	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.38	J/molxK	715.38	Joback Method
cpg	617.50	J/molxK	748.97	Joback Method
cpg	631.73	J/molxK	782.56	Joback Method
cpg	645.08	J/molxK	816.14	Joback Method
cpg	657.56	J/molxK	849.73	Joback Method
cpg	669.17	J/molxK	883.32	Joback Method
cpg	679.92	J/molxK	916.91	Joback Method
dvisc	0.0007768	Paxs	434.58	Joback Method

dvisc	0.0004628	Paxs	481.38	Joback Method
dvisc	0.0003022	Paxs	528.18	Joback Method
dvisc	0.0002115	Paxs	574.98	Joback Method
dvisc	0.0001562	Paxs	621.78	Joback Method
dvisc	0.0001204	Paxs	668.58	Joback Method
dvisc	0.0000960	Paxs	715.38	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=U415079&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

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