

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

Inchi:	InChI=1S/C13H17ClO3/c1-3-16-13(15)5-4-8-17-12-7-6-11(14)9-10(12)2/h6-7,9H,3-5,8H2
InchiKey:	XNKARWLGLZGMGX-UHFFFAOYSA-N
Formula:	C13H17ClO3
SMILES:	CCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]:	256.73

Physical Properties

Property code	Value	Unit	Source
gf	-199.12	kJ/mol	Joback Method
hf	-490.82	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.371		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	669.62	K	Joback Method
tc	876.10	K	Joback Method
tf	412.04	K	Joback Method
vc	0.747	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.56	J/molxK	669.62	Joback Method
cpg	559.43	J/molxK	841.69	Joback Method
cpg	548.46	J/molxK	807.27	Joback Method
cpg	536.69	J/molxK	772.86	Joback Method
cpg	524.12	J/molxK	738.45	Joback Method
cpg	510.74	J/molxK	704.03	Joback Method
cpg	569.61	J/molxK	876.10	Joback Method
dvisc	0.0001213	Paxs	669.62	Joback Method

dvisc	0.0001508	Paxs	626.69	Joback Method
dvisc	0.0001935	Paxs	583.76	Joback Method
dvisc	0.0002584	Paxs	540.83	Joback Method
dvisc	0.0003627	Paxs	497.90	Joback Method
dvisc	0.0005428	Paxs	454.97	Joback Method
dvisc	0.0008835	Paxs	412.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415076&Units=SI

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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