

4-Chlorobutyric acid, 3-ethylphenyl ester

Inchi:	InChI=1S/C12H15ClO2/c1-2-10-5-3-6-11(9-10)15-12(14)7-4-8-13/h3,5-6,9H,2,4,7-8H2,1
InchiKey:	VYWJAMFRRKYCKZ-UHFFFAOYSA-N
Formula:	C12H15ClO2
SMILES:	CCc1cccc(OC(=O)CCCCl)c1
Mol. weight [g/mol]:	226.70

Physical Properties

Property code	Value	Unit	Source
gf	-92.91	kJ/mol	Joback Method
hf	-326.49	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.173		Crippen Method
mvol	175.860	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1728.00		NIST Webbook
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tb	619.34	K	Joback Method
tc	830.22	K	Joback Method
tf	366.02	K	Joback Method
vc	0.672	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.33	J/molxK	619.34	Joback Method
cpg	435.34	J/molxK	654.49	Joback Method
cpg	448.54	J/molxK	689.63	Joback Method
cpg	460.94	J/molxK	724.78	Joback Method
cpg	472.56	J/molxK	759.93	Joback Method
cpg	483.41	J/molxK	795.07	Joback Method
cpg	493.53	J/molxK	830.22	Joback Method
dvisc	0.0015544	Paxs	366.02	Joback Method

dvisc	0.0008929	Paxs	408.24	Joback Method
dvisc	0.0005690	Paxs	450.46	Joback Method
dvisc	0.0003918	Paxs	492.68	Joback Method
dvisc	0.0002861	Paxs	534.90	Joback Method
dvisc	0.0002188	Paxs	577.12	Joback Method
dvisc	0.0001735	Paxs	619.34	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=U360642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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