

4-Chlorobutyric acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C11H13ClO3/c1-14-9-4-6-10(7-5-9)15-11(13)3-2-8-12/h4-7H,2-3,8H2,1H3
InchiKey:	JBOBRZWEFOHJFK-UHFFFAOYSA-N
Formula:	C11H13ClO3
SMILES:	COc1ccc(OC(=O)CCCCl)cc1
Mol. weight [g/mol]:	228.67

Physical Properties

Property code	Value	Unit	Source
gf	-206.33	kJ/mol	Joback Method
hf	-438.07	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.620		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinqol	1730.00		NIST Webbook
tb	618.88	K	Joback Method
tc	830.85	K	Joback Method
tf	376.98	K	Joback Method
vc	0.634	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.18	J/molxK	618.88	Joback Method
cpg	410.26	J/molxK	654.21	Joback Method
cpg	422.61	J/molxK	689.54	Joback Method
cpg	434.21	J/molxK	724.87	Joback Method
cpg	445.07	J/molxK	760.19	Joback Method
cpg	455.20	J/molxK	795.52	Joback Method
cpg	464.60	J/molxK	830.85	Joback Method
dvisc	0.0011984	Paxs	376.98	Joback Method
dvisc	0.0007196	Paxs	417.30	Joback Method

dvisc	0.0004728	Paxs	457.61	Joback Method
dvisc	0.0003324	Paxs	497.93	Joback Method
dvisc	0.0002464	Paxs	538.25	Joback Method
dvisc	0.0001905	Paxs	578.56	Joback Method
dvisc	0.0001522	Paxs	618.88	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=U307603&Units=SI

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
log_p:	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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