4-Chlorobutyric acid, cyclohexyl ester

Inchi: InChI=1S/C10H17ClO2/c11-8-4-7-10(12)13-9-5-2-1-3-6-9/h9H,1-8H2
InchiKey: JFVJNSGGFOFSRK-UHFFFAOYSA-N
Formula: C10H17ClO2
SMILES: O=C(CCCCl)OC1CCCCC1
Mol. weight [g/mol]: 204.69

Physical Properties

Property code	Value	Unit	Source
gf	-188.08	kJ/mol	Joback Method
hf	-455.95	kJ/mol	Joback Method
hfus	20.48	kJ/mol	Joback Method
hvap	51.82	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.881		Crippen Method
mcvol	160.580	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1490.00		NIST Webbook
tb	561.47	K	Joback Method
tc	771.44	K	Joback Method
tf	311.92	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.64	J/mol×K	561.47	Joback Method
cpg	403.61	J/mol×K	596.46	Joback Method
cpg	419.65	J/mol×K	631.46	Joback Method
cpg	434.77	J/mol×K	666.45	Joback Method
cpg	448.99	J/mol×K	701.45	Joback Method
cpg	462.33	J/mol×K	736.44	Joback Method
cpg	474.81	J/mol×K	771.44	Joback Method
dvisc	0.0036096	Pa×s	311.92	Joback Method
dvisc	0.0017523	Pa×s	353.51	Joback Method

dvisc	0.0009905	Pa×s	395.10	Joback Method
dvisc	0.0006241	Pa×s	436.70	Joback Method
dvisc	0.0004262	Pa×s	478.29	Joback Method
dvisc	0.0003093	Pa×s	519.88	Joback Method
dvisc	0.0002354	Pa×s	561.47	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=U357768&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