4-Chlorobutyric acid, cyclohexylmethyl ester

Inchi: InChI=1S/C11H19ClO2/c12-8-4-7-11(13)14-9-10-5-2-1-3-6-10/h10H,1-9H2
InchiKey: RHJHMXCSXWBNAI-UHFFFAOYSA-N
Formula: C11H19ClO2
SMILES: O=C(CCCCl)OCC1CCCCC1
Mol. weight [g/mol]: 218.72

Physical Properties

Property code	Value	Unit	Source
gf	-179.66	kJ/mol	Joback Method
hf	-476.59	kJ/mol	Joback Method
hfus	23.07	kJ/mol	Joback Method
hvap	54.05	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.129		Crippen Method
mcvol	174.670	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	584.35	K	Joback Method
tc	791.01	K	Joback Method
tf	323.19	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.25	J/mol×K	584.35	Joback Method
cpg	514.59	J/mol×K	756.56	Joback Method
cpg	500.78	J/mol×K	722.12	Joback Method
cpg	486.07	J/mol×K	687.68	Joback Method
cpg	470.41	J/mol×K	653.24	Joback Method
cpg	453.81	J/mol×K	618.79	Joback Method
cpg	527.50	J/mol×K	791.01	Joback Method
dvisc	0.0002119	Pa×s	584.35	Joback Method

dvisc	0.0002795	Pa×s	540.82	Joback Method
dvisc	0.0003870	Pa×s	497.30	Joback Method
dvisc	0.0005702	Pa×s	453.77	Joback Method
dvisc	0.0009123	Pa×s	410.24	Joback Method
dvisc	0.0016320	Pa×s	366.72	Joback Method
dvisc	0.0034145	Pa×s	323.19	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=U357770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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