Glycine, 2-cyclohexyl-N-(3-chloropropoxycarbonyl)-, isobutyl ester

Inchi: InChI=1S/C16H28ClNO4/c1-12(2)11-22-15(19)14(13-7-4-3-5-8-13)18-16(20)21-10-6-9-1

InchiKey: FCSFTORRKVXTLU-UHFFFAOYSA-N

Formula: C16H28ClNO4

SMILES: CC(C)COC(=O)C(NC(=O)OCCCCl)C1CCCCC1

Mol. weight [g/mol]: 333.85

Physical Properties

Property code	Value	Unit	Source
gf	-286.97	kJ/mol	Joback Method
hf	-781.68	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	80.00	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.490		Crippen Method
mcvol	262.540	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	824.33	K	Joback Method
tc	1031.93	K	Joback Method
tf	474.36	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.67	J/mol×K	824.33	Joback Method
cpg	837.13	J/mol×K	858.93	Joback Method
cpg	852.31	J/mol×K	893.53	Joback Method
cpg	866.22	J/mol×K	928.13	Joback Method
cpg	878.88	J/mol×K	962.73	Joback Method
cpg	890.30	J/mol×K	997.33	Joback Method
cpg	900.52	J/mol×K	1031.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U392343&Units=SI

Legend

cpg:	Ideal gas heat capacity
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