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

Inchi: InChI=1S/C16H28ClNO4/c1-2-3-11-21-15(19)14(13-8-5-4-6-9-13)18-16(20)22-12-7-10-1
InchiKey: MSMPHNKADJWGSM-UHFFFAOYSA-N
Formula: C16H28ClNO4
SMILES: CCCCOC(=O)C(NC(=O)OCCCCl)C1CCCCC1
Mol. weight [g/mol]: 333.85

Physical Properties

Property code	Value	Unit	Source
gf	-284.53	kJ/mol	Joback Method
hf	-776.40	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.634		Crippen Method
mcvol	262.540	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tb	824.77	K	Joback Method
tc	1030.03	K	Joback Method
tf	489.36	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.14	J/mol×K	824.77	Joback Method
cpg	836.43	J/mol×K	858.98	Joback Method
cpg	851.47	J/mol×K	893.19	Joback Method
cpg	865.28	J/mol×K	927.40	Joback Method
cpg	877.88	J/mol×K	961.61	Joback Method
cpg	889.28	J/mol×K	995.82	Joback Method
cpg	899.51	J/mol×K	1030.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392336&Units=SI
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

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