

Glycine, 2-cyclohexyl-N-ethoxycarbonyl-, octadecyl ester

Inchi:	InChI=1S/C29H55NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-25-34-28(31)27(3
InchiKey:	NJJUNYWHCRZBQW-UHFFFAOYSA-N
Formula:	C29H55NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)OCC)C1CCCCC1
Mol. weight [g/mol]:	481.75

Physical Properties

Property code	Value	Unit	Source
gf	-163.14	kJ/mol	Joback Method
hf	-1028.98	kJ/mol	Joback Method
hfus	69.85	kJ/mol	Joback Method
hvap	104.94	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	8.486		Crippen Method
mvol	433.470	ml/mol	McGowan Method
pc	736.82	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	1084.78	K	Joback Method
tc	1345.76	K	Joback Method
tf	605.95	K	Joback Method
vc	1.669	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1598.94	J/molxK	1084.78	Joback Method
cpg	1618.59	J/molxK	1128.28	Joback Method
cpg	1635.73	J/molxK	1171.77	Joback Method
cpg	1650.48	J/molxK	1215.27	Joback Method
cpg	1662.94	J/molxK	1258.77	Joback Method
cpg	1673.22	J/molxK	1302.26	Joback Method
cpg	1681.45	J/molxK	1345.76	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=U383094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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