Glycine, 2-cyclohexyl-N-(2,3,4-trifluorobenzoyl)-, octyl ester

Inchi: InChI=1S/C23H32F3NO3/c1-2-3-4-5-6-10-15-30-23(29)21(16-11-8-7-9-12-16)27-22(28)1

InchiKey: FYALDWWLNRZDES-UHFFFAOYSA-N

Formula: C23H32F3NO3

SMILES: CCCCCCCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1F)C1CCCCC1

Mol. weight [g/mol]: 427.50

Physical Properties

Property code	Value	Unit	Source
gf	-609.57	kJ/mol	Joback Method
hf	-1159.13	kJ/mol	Joback Method
hfus	55.24	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	5.686		Crippen Method
mcvol	324.610	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	964.51	K	Joback Method
tc	1181.99	K	Joback Method
tf	581.85	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.61	J/mol×K	964.51	Joback Method
cpg	1118.83	J/mol×K	1000.76	Joback Method
cpg	1132.57	J/mol×K	1037.00	Joback Method
cpg	1144.90	J/mol×K	1073.25	Joback Method
cpg	1155.85	J/mol×K	1109.50	Joback Method
cpg	1165.48	J/mol×K	1145.74	Joback Method
cpg	1173.84	J/mol×K	1181.99	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=U383125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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