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

Inchi: InChI=1S/C17H20F3NO3/c1-2-24-17(23)15(10-6-4-3-5-7-10)21-16(22)11-8-9-12(18)14(2

InchiKey: QXYMYRACOQGFQG-UHFFFAOYSA-N

Formula: C17H20F3NO3

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

Mol. weight [g/mol]: 343.34

Physical Properties

Property code	Value	Unit	Source
gf	-660.09	kJ/mol	Joback Method
hf	-1035.29	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	77.63	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.346		Crippen Method
mcvol	240.070	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
tb	827.23	K	Joback Method
tc	1038.28	K	Joback Method
tf	514.23	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.63	J/mol×K	827.23	Joback Method
cpg	763.24	J/mol×K	862.41	Joback Method
cpg	776.64	J/mol×K	897.58	Joback Method
cpg	788.85	J/mol×K	932.76	Joback Method
cpg	799.90	J/mol×K	967.93	Joback Method
cpg	809.81	J/mol×K	1003.11	Joback Method
cpg	818.62	J/mol×K	1038.28	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=U383120&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