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

Inchi: InChI=1S/C19H24F3NO3/c1-11(2)10-26-19(25)17(12-6-4-3-5-7-12)23-18(24)13-8-9-14(2
InchiKey: AJLCVEFOKGQVAU-UHFFFAOYSA-N
Formula: C19H24F3NO3
SMILES: CC(C)COC(=O)C(NC(=O)c1ccc(F)c(F)c1F)C1CCCCC1
Mol. weight [g/mol]: 371.39

Physical Properties

Property code	Value	Unit	Source
gf	-645.69	kJ/mol	Joback Method
hf	-1081.85	kJ/mol	Joback Method
hfus	41.35	kJ/mol	Joback Method
hvap	81.69	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	3.982		Crippen Method
mcvol	268.250	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	872.55	K	Joback Method
tc	1084.67	K	Joback Method
tf	521.77	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.89	J/mol×K	872.55	Joback Method
cpg	879.84	J/mol×K	907.90	Joback Method
cpg	893.48	J/mol×K	943.26	Joback Method
cpg	905.83	J/mol×K	978.61	Joback Method
cpg	916.94	J/mol×K	1013.96	Joback Method
cpg	926.84	J/mol×K	1049.31	Joback Method
cpg	935.56	J/mol×K	1084.67	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=U383122&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