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

Inchi: InChI=1S/C18H22F3NO3/c1-2-10-25-18(24)16(11-6-4-3-5-7-11)22-17(23)12-8-9-13(19)1

InchiKey: XRTMSWBHVZHBOY-UHFFFAOYSA-N

Formula: C18H22F3NO3

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

Mol. weight [g/mol]: 357.37

Physical Properties

Property code	Value	Unit	Source
gf	-651.67	kJ/mol	Joback Method
hf	-1055.93	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	3.736		Crippen Method
mcvol	254.160	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	850.11	K	Joback Method
tc	1060.35	K	Joback Method
tf	525.50	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.12	J/mol×K	850.11	Joback Method
cpg	820.85	J/mol×K	885.15	Joback Method
cpg	834.34	J/mol×K	920.19	Joback Method
cpg	846.61	J/mol×K	955.23	Joback Method
cpg	857.70	J/mol×K	990.27	Joback Method
cpg	867.63	J/mol×K	1025.31	Joback Method
cpg	876.44	J/mol×K	1060.35	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=U383121&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