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

Inchi: InChI=1S/C20H26F3NO3/c1-2-3-7-12-27-20(26)18(13-8-5-4-6-9-13)24-19(25)14-10-11-1

InchiKey: IQFXGTHYWBCBJG-UHFFFAOYSA-N

Formula: C20H26F3NO3

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

Mol. weight [g/mol]: 385.42

Physical Properties

Property code	Value	Unit	Source
gf	-634.83	kJ/mol	Joback Method
hf	-1097.21	kJ/mol	Joback Method
hfus	47.47	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	4.516		Crippen Method
mcvol	282.340	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook
tb	895.87	K	Joback Method
tc	1106.58	K	Joback Method
tf	548.04	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.30	J/mol×K	895.87	Joback Method
cpg	938.23	J/mol×K	930.99	Joback Method
cpg	951.83	J/mol×K	966.11	Joback Method
cpg	964.16	J/mol×K	1001.23	Joback Method
cpg	975.25	J/mol×K	1036.35	Joback Method
cpg	985.13	J/mol×K	1071.47	Joback Method
cpg	993.84	J/mol×K	1106.58	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=U383124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume