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

Inchi: InChI=1S/C19H24F3NO3/c1-2-3-11-26-19(25)17(12-7-5-4-6-8-12)23-18(24)13-9-10-14(2

InchiKey: NSLTZIGRKJXRMU-UHFFFAOYSA-N

Formula: C19H24F3NO3

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

Mol. weight [g/mol]: 371.39

Physical Properties

Property code	Value	Unit	Source
gf	-643.25	kJ/mol	Joback Method
hf	-1076.57	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.126		Crippen Method
mcvol	268.250	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	872.99	K	Joback Method
tc	1083.10	K	Joback Method
tf	536.77	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.37	J/mol×K	872.99	Joback Method
cpg	879.20	J/mol×K	908.01	Joback Method
cpg	892.76	J/mol×K	943.03	Joback Method
cpg	905.07	J/mol×K	978.04	Joback Method
cpg	916.16	J/mol×K	1013.06	Joback Method
cpg	926.08	J/mol×K	1048.08	Joback Method
cpg	934.85	J/mol×K	1083.10	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=U383123&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