l-Phenylalanine, N-(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C17H14F3NO3/c1-24-17(23)13(9-10-5-3-2-4-6-10)21-16(22)11-7-8-12(18)15(2

InchiKey: VRJONYFRIFFQGQ-UHFFFAOYSA-N

Formula: C17H14F3NO3

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 337.29

Physical Properties

Property code	Value	Unit	Source
gf	-572.13	kJ/mol	Joback Method
hf	-853.08	kJ/mol	Joback Method
hfus	41.90	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	2.618		Crippen Method
mcvol	227.170	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2123.00		NIST Webbook
tb	834.36	K	Joback Method
tc	1049.87	K	Joback Method
tf	533.27	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.59	J/mol×K	834.36	Joback Method
cpg	671.32	J/mol×K	870.28	Joback Method
cpg	682.02	J/mol×K	906.20	Joback Method
cpg	691.74	J/mol×K	942.12	Joback Method
cpg	700.49	J/mol×K	978.04	Joback Method
cpg	708.31	J/mol×K	1013.95	Joback Method
cpg	715.25	J/mol×K	1049.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299633&Units=SI
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

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