l-Phenylalanine, N-(2-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C18H16F3NO3/c1-25-17(24)15(11-12-7-3-2-4-8-12)22-16(23)13-9-5-6-10-14(1

InchiKey: DFYVDBGYKDQXTB-UHFFFAOYSA-N

Formula: C18H16F3NO3

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 351.32

Physical Properties

Property code	Value	Unit	Source
gf	-541.61	kJ/mol	Joback Method
hf	-859.53	kJ/mol	Joback Method
hfus	37.86	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.219		Crippen Method
mcvol	241.260	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
tb	844.05	K	Joback Method
tc	1064.30	K	Joback Method
tf	521.92	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.35	J/mol×K	844.05	Joback Method
cpg	731.65	J/mol×K	880.76	Joback Method
cpg	742.86	J/mol×K	917.47	Joback Method
cpg	753.07	J/mol×K	954.17	Joback Method
cpg	762.35	J/mol×K	990.88	Joback Method
cpg	770.78	J/mol×K	1027.59	Joback Method
cpg	778.42	J/mol×K	1064.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299688&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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