l-Phenylalanine, N-(O-anisoyl)-, methyl ester

Inchi: InChI=1S/C18H19NO4/c1-22-16-11-7-6-10-14(16)17(20)19-15(18(21)23-2)12-13-8-4-3-5
InchiKey: SXNQWRUVXCKZKG-UHFFFAOYSA-N
Formula: C18H19NO4
SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1ccccc1OC
Mol. weight [g/mol]: 313.35

Physical Properties

Property code	Value	Unit	Source
gf	-65.02	kJ/mol	Joback Method
hf	-394.67	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	85.24	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.209		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	871.89	K	Joback Method
tc	1103.42	K	Joback Method
tf	539.96	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.11	J/mol×K	871.89	Joback Method
cpg	735.12	J/mol×K	910.48	Joback Method
cpg	746.83	J/mol×K	949.07	Joback Method
cpg	757.26	J/mol×K	987.65	Joback Method
cpg	766.47	J/mol×K	1026.24	Joback Method
cpg	774.48	J/mol×K	1064.83	Joback Method
cpg	781.34	J/mol×K	1103.42	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=U299756&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