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
hf	-477.42	kJ/mol	Cheméo Relay (1.0)
hfus	37.22	kJ/mol	Joback Method
hvap	111.77	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.54		Cheméo Relay (1.0)
logp	2.209		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	652.42	K	Cheméo Relay (1.0)
tf	374.54	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299756&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point