l-Phenylalanine-, N-(p-toluoyl)-, methyl ester

Inchi: InChI=1S/C18H19NO3/c1-13-8-10-15(11-9-13)17(20)19-16(18(21)22-2)12-14-6-4-3-5-7-
InchiKey: PSSDDHSCEICJEX-UHFFFAOYSA-N
Formula: C18H19NO3
SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 297.35

Physical Properties

Property code	Value	Unit	Source
gf	39.98	kJ/mol	Joback Method
hf	-262.45	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	82.83	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.509		Crippen Method
mcvol	235.950	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	849.47	K	Joback Method
tc	1082.95	K	Joback Method
tf	517.73	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.62	J/mol×K	849.47	Joback Method
cpg	709.30	J/mol×K	888.38	Joback Method
cpg	721.74	J/mol×K	927.30	Joback Method
cpg	732.99	J/mol×K	966.21	Joback Method
cpg	743.11	J/mol×K	1005.12	Joback Method
cpg	752.16	J/mol×K	1044.03	Joback Method
cpg	760.21	J/mol×K	1082.95	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=U299645&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