l-Phenylalanine, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C18H25NO3/c1-22-18(21)16(13-15-9-3-2-4-10-15)19-17(20)12-11-14-7-5-6-8-
InchiKey: QFAPOGGWKDCBDP-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: COC(=O)C(Cc1ccccc1)NC(=O)CCC1CCCC1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
gf	-26.25	kJ/mol	Joback Method
hf	-427.03	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	80.14	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	2.857		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2307.00		NIST Webbook
rinpol	2307.00		NIST Webbook
tb	833.09	K	Joback Method
tc	1055.32	K	Joback Method
tf	489.69	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.79	J/mol×K	833.09	Joback Method
cpg	799.20	J/mol×K	870.13	Joback Method
cpg	814.29	J/mol×K	907.17	Joback Method
cpg	828.12	J/mol×K	944.21	Joback Method
cpg	840.75	J/mol×K	981.25	Joback Method
cpg	852.24	J/mol×K	1018.29	Joback Method
cpg	862.66	J/mol×K	1055.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299656&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