l-Phenylalanine, N-capryloyl-, methyl ester

Inchi: InChI=1S/C18H27NO3/c1-3-4-5-6-10-13-17(20)19-16(18(21)22-2)14-15-11-8-7-9-12-15/h
InchiKey: OUCOUUMRVGYPMW-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCCCCCCC(=O)NC(Cc1ccccc1)C(=O)OC
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-62.80	kJ/mol	Joback Method
hf	-487.51	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.247		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	817.81	K	Joback Method
tc	1021.72	K	Joback Method
tf	478.79	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.02	J/mol×K	817.81	Joback Method
cpg	807.59	J/mol×K	851.80	Joback Method
cpg	822.09	J/mol×K	885.78	Joback Method
cpg	835.54	J/mol×K	919.77	Joback Method
cpg	848.00	J/mol×K	953.75	Joback Method
cpg	859.49	J/mol×K	987.74	Joback Method
cpg	870.06	J/mol×K	1021.72	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=U299728&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