l-Phenylalanine, N-butyryl-, methyl ester

Inchi: InChI=1S/C14H19NO3/c1-3-7-13(16)15-12(14(17)18-2)10-11-8-5-4-6-9-11/h4-6,8-9,12H
InchiKey: RBBWRWZNNKHWQT-UHFFFAOYSA-N
Formula: C14H19NO3
SMILES: CCCC(=O)NC(Cc1ccccc1)C(=O)OC
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-96.48	kJ/mol	Joback Method
hf	-404.95	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	70.98	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.687		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1819.00		NIST Webbook
rinpol	1819.00		NIST Webbook
tb	726.29	K	Joback Method
tc	936.72	K	Joback Method
tf	433.71	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.61	J/mol×K	726.29	Joback Method
cpg	583.12	J/mol×K	761.36	Joback Method
cpg	596.63	J/mol×K	796.43	Joback Method
cpg	609.18	J/mol×K	831.51	Joback Method
cpg	620.80	J/mol×K	866.58	Joback Method
cpg	631.52	J/mol×K	901.65	Joback Method
cpg	641.37	J/mol×K	936.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308817&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