

L-phenylalanine, n-(4-butylbenzoyl)-, methyl ester

Inchi:	InChI=1S/C21H25NO3/c1-3-4-8-16-11-13-18(14-12-16)20(23)22-19(21(24)25-2)15-17-9
InchiKey:	AXCCLNAVUHVWCT-UHFFFAOYSA-N
Formula:	C21H25NO3
SMILES:	CCCCc1ccc(C(=O)NC(Cc2ccccc2)C(=O)OC)cc1
Mol. weight [g/mol]:	339.43

Physical Properties

Property code	Value	Unit	Source
af	0.8211		Cheméo Relay (1.0)
gf	65.24	kJ/mol	Joback Method
hf	-441.79	kJ/mol	Cheméo Relay (1.0)
hfus	43.80	kJ/mol	Joback Method
hvap	118.55	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-4.87		Cheméo Relay (1.0)
logp	3.543		Crippen Method
mcvol	278.220	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2926.00		NIST Webbook
rinpol	2926.00		NIST Webbook
tb	669.87	K	Cheméo Relay (1.0)
tc	931.39	K	Cheméo Relay (1.0)
tf	349.22	K	Cheméo Relay (1.0)
vc	0.990	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.91	J/mol×K	918.11	Joback Method
cpg	881.91	J/mol×K	955.98	Joback Method
cpg	894.66	J/mol×K	993.85	Joback Method
cpg	906.22	J/mol×K	1031.73	Joback Method
cpg	916.65	J/mol×K	1069.60	Joback Method
cpg	926.02	J/mol×K	1107.47	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299697&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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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