

L-Alanine, N-(4-butylbenzoyl)-, methyl ester

Inchi:	InChI=1S/C15H21NO3/c1-4-5-6-12-7-9-13(10-8-12)14(17)16-11(2)15(18)19-3/h7-11H,4-
InchiKey:	SHIVHQBYQKEZEA-UHFFFAOYSA-N
Formula:	C15H21NO3
SMILES:	CCCCc1ccc(C(=O)NC(C)C(=O)OC)cc1
Mol. weight [g/mol]:	263.34

Physical Properties

Property code	Value	Unit	Source
hfus	34.22	kJ/mol	Joback Method
ie	8.62	eV	Cheméo Relay (1.0)
logp	2.321		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
rinpol	2074.00		NIST Webbook
tb	596.35	K	Cheméo Relay (1.0)
tf	343.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.01	J/mol×K	754.15	Joback Method
cpg	636.72	J/mol×K	788.95	Joback Method
cpg	650.44	J/mol×K	823.75	Joback Method
cpg	663.19	J/mol×K	858.55	Joback Method
cpg	675.00	J/mol×K	893.35	Joback Method
cpg	685.89	J/mol×K	928.15	Joback Method
cpg	695.89	J/mol×K	962.94	Joback Method

Sources

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>
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=U299692&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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