

D-Alanine, N-(4-butylbenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C26H43NO3/c1-4-6-8-9-10-11-12-13-14-15-21-30-26(29)22(3)27-25(28)24-19
InchiKey:	KIPISLLURSFBED-UHFFFAOYSA-N
Formula:	C26H43NO3
SMILES:	CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	417.62

Physical Properties

Property code	Value	Unit	Source
gf	-5.07	kJ/mol	Joback Method
hf	-664.10	kJ/mol	Joback Method
hfus	62.71	kJ/mol	Joback Method
hvap	98.36	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	6.612		Crippen Method
mvol	372.430	ml/mol	McGowan Method
pc	936.35	kPa	Joback Method
rinpol	3227.00		NIST Webbook
rinpol	3227.00		NIST Webbook
tb	1005.83	K	Joback Method
tc	1232.32	K	Joback Method
tf	581.47	K	Joback Method
vc	1.442	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.93	J/molxK	1005.83	Joback Method
cpg	1293.41	J/molxK	1043.58	Joback Method
cpg	1309.41	J/molxK	1081.33	Joback Method
cpg	1324.01	J/molxK	1119.08	Joback Method
cpg	1337.28	J/molxK	1156.83	Joback Method
cpg	1349.30	J/molxK	1194.57	Joback Method
cpg	1360.14	J/molxK	1232.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U354103&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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