

«beta»-Alanine, N-(4-methylbezoyl)-, tetradecyl ester

Inchi:	InChI=1S/C25H41NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-21-29-24(27)19-20-26-25(28)23
InchiKey:	JUJSDBCXCAPAIE-UHFFFAOYSA-N
Formula:	C25H41NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	403.60

Physical Properties

Property code	Value	Unit	Source
gf	-11.05	kJ/mol	Joback Method
hf	-638.18	kJ/mol	Joback Method
hfus	63.64	kJ/mol	Joback Method
hvap	96.52	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.359		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
tb	983.39	K	Joback Method
tc	1204.19	K	Joback Method
tf	585.20	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.01	J/mol×K	983.39	Joback Method
cpg	1230.24	J/mol×K	1020.19	Joback Method
cpg	1246.07	J/mol×K	1056.99	Joback Method
cpg	1260.58	J/mol×K	1093.79	Joback Method
cpg	1273.84	J/mol×K	1130.59	Joback Method
cpg	1285.91	J/mol×K	1167.39	Joback Method
cpg	1296.85	J/mol×K	1204.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321611&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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