

«beta»-Alanine, N-(3-methoxybenzoyl)-, isoheyl ester

Inchi:	InChI=1S/C17H25NO4/c1-13(2)6-5-11-22-16(19)9-10-18-17(20)14-7-4-8-15(12-14)21-3/
InchiKey:	YJQMFDUDNRHR-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	COc1cccc(C(=O)NCCC(=O)OCCCC(C)C)c1
Mol. weight [g/mol]:	307.38

Physical Properties

Property code	Value	Unit	Source
gf	-185.85	kJ/mol	Joback Method
hf	-610.56	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.794		Crippen Method
mvol	251.490	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	822.33	K	Joback Method
tc	1027.63	K	Joback Method
tf	502.27	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.10	J/mol×K	822.33	Joback Method
cpg	776.91	J/mol×K	856.55	Joback Method
cpg	790.62	J/mol×K	890.76	Joback Method
cpg	803.26	J/mol×K	924.98	Joback Method
cpg	814.83	J/mol×K	959.20	Joback Method
cpg	825.37	J/mol×K	993.42	Joback Method
cpg	834.88	J/mol×K	1027.63	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=U321708&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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