

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

Inchi:	InChI=1S/C19H29NO4/c1-3-4-5-6-7-8-14-24-18(21)12-13-20-19(22)16-10-9-11-17(15-16)
InchiKey:	HEVAFTFLJRNSHF-UHFFFAOYSA-N
Formula:	C19H29NO4
SMILES:	CCCCCCCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	335.44

Physical Properties

Property code	Value	Unit	Source
gf	-166.57	kJ/mol	Joback Method
hf	-646.56	kJ/mol	Joback Method
hfus	49.29	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.719		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2757.00		NIST Webbook
tb	868.53	K	Joback Method
tc	1072.52	K	Joback Method
tf	539.81	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.84	J/mol×K	868.53	Joback Method
cpg	892.93	J/mol×K	902.53	Joback Method
cpg	906.88	J/mol×K	936.53	Joback Method
cpg	919.70	J/mol×K	970.53	Joback Method
cpg	931.42	J/mol×K	1004.53	Joback Method
cpg	942.05	J/mol×K	1038.52	Joback Method
cpg	951.64	J/mol×K	1072.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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