

Beta-alanine, n-benzyl-n-carboxymethyl, diethyl ester

Other names:	ethyl N-(2-ethoxy-2-oxoethyl)-N-(phenylmethyl)-«beta»-alaninate
Inchi:	InChI=1S/C16H23NO4/c1-3-20-15(18)10-11-17(13-16(19)21-4-2)12-14-8-6-5-7-9-14/h5-
InchiKey:	JWYHGTSTWMQTHS-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CCOC(=O)CCN(CC(=O)OCC)Cc1ccccc1
Mol. weight [g/mol]:	293.36
CAS:	795-18-6

Physical Properties

Property code	Value	Unit	Source
gf	-160.81	kJ/mol	Joback Method
hf	-559.11	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.005		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
tb	757.18	K	Joback Method
tc	956.65	K	Joback Method
tf	473.29	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.82	J/molxK	757.18	Joback Method
cpg	705.14	J/molxK	790.42	Joback Method
cpg	719.44	J/molxK	823.67	Joback Method
cpg	732.75	J/molxK	856.91	Joback Method
cpg	745.09	J/molxK	890.16	Joback Method
cpg	756.49	J/molxK	923.40	Joback Method
cpg	766.98	J/molxK	956.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C795186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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