

«beta»-Alanine, N-(2-chlorobenzoyl)-,hexyl ester

Inchi:	InChI=1S/C16H22ClNO3/c1-2-3-4-7-12-21-15(19)10-11-18-16(20)13-8-5-6-9-14(13)17/h
InchiKey:	UNIHSLUFSWZHBU-UHFFFAOYSA-N
Formula:	C16H22ClNO3
SMILES:	CCCCCOC(=O)CCNC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	311.80

Physical Properties

Property code	Value	Unit	Source
gf	-98.76	kJ/mol	Joback Method
hf	-468.16	kJ/mol	Joback Method
hfus	44.53	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.583		Crippen Method
mvol	243.770	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	814.90	K	Joback Method
tc	1022.88	K	Joback Method
tf	513.69	K	Joback Method
vc	0.938	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.86	J/mol×K	814.90	Joback Method
cpg	716.54	J/mol×K	849.56	Joback Method
cpg	729.23	J/mol×K	884.23	Joback Method
cpg	740.98	J/mol×K	918.89	Joback Method
cpg	751.80	J/mol×K	953.55	Joback Method
cpg	761.74	J/mol×K	988.22	Joback Method
cpg	770.82	J/mol×K	1022.88	Joback Method

Sources

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=U321576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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