

DL-Alanine, N-benzoyl-N-(3,4-dichlorophenyl)-, ethyl ester

Other names:	DL-Alanine, N-benzoyl-N-(3,4-dichlorophenyl)-, ethyl ester Alanine, N-benzoyl-N-(3,4-dichlorophenyl)-, ethyl ester, DL-Endaven Ethyl 2-(N-benzoyl-3,4-dichloroanilino)propionate Ethyl 2-[benzoyl(3,4-dichlorophenyl)amino]propionate Ethyl 2-[N-(3,4-dichlorophenyl)benzamido]propionate FX 2182 Suffix Propionic acid, 2-(N-benzoyl-N-(3,4-dichlorophenyl))amino-, ethyl ester N-Benzoyl-N-(3,4-dichlorophenyl)-dl-alanine ethyl ester Ethyl N-benzoyl-N-(3,4-dichlorophenyl)-2-aminopropionate SD 30,053 Suffix 25 Alanine, N-benzoyl-N-(3,4-dichlorophenyl)-, ethyl ester Propionic acid, 2-(N-benzoyl-N-(3,4-dichlorophenyl))amino-, ethyl ester, (.+/-.)-ethyl N-benzoyl-N-(3,4-dichlorophenyl)-DL-alaninate
Inchi:	InChI=1S/C18H17Cl2NO3/c1-3-24-18(23)12(2)21(14-9-10-15(19)16(20)11-14)17(22)13-
InchiKey:	SLCGUGMPSUYJAY-UHFFFAOYSA-N
Formula:	C18H17Cl2NO3
SMILES:	CCOC(=O)C(C)N(C(=O)c1ccccc1)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	366.24

Physical Properties

Property code	Value	Unit	Source
af	0.7357		Cheméo Relay (1.0)
hfus	41.96	kJ/mol	Joback Method
hvap	108.38	kJ/mol	Cheméo Relay (1.0)
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-5.12		Cheméo Relay (1.0)
logp	4.592		Crippen Method
mcvol	260.430	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
tb	657.09	K	Cheméo Relay (1.0)
tc	941.77	K	Cheméo Relay (1.0)
tf	350.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.73	J/mol×K	891.58	Joback Method
cpg	738.61	J/mol×K	931.22	Joback Method
cpg	749.31	J/mol×K	970.86	Joback Method
cpg	758.92	J/mol×K	1010.50	Joback Method
cpg	767.50	J/mol×K	1050.14	Joback Method
cpg	775.12	J/mol×K	1089.78	Joback Method
cpg	781.85	J/mol×K	1129.42	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C22212551

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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