Benzoylprop-ethyl

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)13-1
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
CAS:	22212-55-1

Physical Properties

Property code	Value	Unit	Source
gf	27.88	kJ/mol	Joback Method
hf	-291.34	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.592		Crippen Method
mcvol	260.430	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
tb	891.58	K	Joback Method
tc	1129.42	K	Joback Method
tf	343.27 ± 0.20	K	NIST Webbook
vc	0.968	m3/kmol	Joback Method

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
hfust	27.06	kJ/mol	341.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22212551&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
hfust: Enthalpy of fusion at a given temperature
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