Glycine, n-(chloroacetyl)-n-(2,6-diethylphenyl)-, ethyl ester

Othernames: Antor
Bay NNT 6867
N-Chloroacetyl-N-(2,6-diethylphenyl)glycine ethyl ester
Diethacine-ethyl
Diethatyl-ethyl
Ethyl N-chloroacetyl-2,6-diethylanilinoacetate
Ethyl N-(2,6-diethylphenyl)-N-(chloroacetyl)aminoacetate
H 22234
Hercules 22234
Nevirex G
ethyl N-(chloroacetyl)-N-(2,6-diethylphenyl)glycinate

Inchi: InChI=1S/C16H22ClNO3/c1-4-12-8-7-9-13(5-2)16(12)18(14(19)10-17)11-15(20)21-6-3/h

InchiKey: WFKSADNZWSKCRZ-UHFFFAOYSA-N

Formula: C16H22ClNO3

SMILES: CCOC(=O)CN(C(=O)CCl)c1c(CC)cccc1CC

Mol. weight [g/mol]: 311.81

Physical Properties

Property code	Value	Unit	Source
hfus	42.06	kJ/mol	Joback Method
hvap	90.40	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.59		Cheméo Relay (1.0)
logp	2.946		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
tf	319.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.44	J/mol×K	782.15	Joback Method
cpg	701.81	J/mol×K	816.42	Joback Method
cpg	715.21	J/mol×K	850.69	Joback Method
cpg	727.67	J/mol×K	884.95	Joback Method
cpg	739.22	J/mol×K	919.22	Joback Method

cpg	749.89	J/mol×K	953.49	Joback Method
cpg	759.71	J/mol×K	987.76	Joback Method
hfust	23.84	kJ/mol	318.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38727558&Units=SI

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

Legend

cpg: Ideal gas heat capacity
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
tf: Normal melting (fusion) point