N-CHLOROACETYL-L-TYROSINE

Other names: N-Chloroacetyl-L-tyrosine
L-Tyrosine, N-(chloroacetyl)-
Inchi: InChI=1S/C11H12ClNO4/c12-6-10(15)13-9(11(16)17)5-7-1-3-8(14)4-2-7/h1-4,9,14H,5-6H
InchiKey: GDOGSOZOUAVIFX-VIFPVBQESA-N
Formula: C11H12ClNO4
SMILES: O=C(CCl)N[C@@H](Cc1ccc(O)cc1)C(=O)O
Mol. weight [g/mol]: 257.67

Physical Properties

Property code	Value	Unit	Source
hfus	37.13	kJ/mol	Joback Method
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)
logp	0.743		Crippen Method
mcvol	179.190	ml/mol	McGowan Method
tf	417.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.14	J/mol×K	845.46	Joback Method
cpg	507.81	J/mol×K	882.14	Joback Method
cpg	516.04	J/mol×K	918.82	Joback Method
cpg	523.92	J/mol×K	955.50	Joback Method
cpg	531.53	J/mol×K	992.18	Joback Method
cpg	538.97	J/mol×K	1028.86	Joback Method
cpg	546.31	J/mol×K	1065.54	Joback Method

Sources

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=C1145568
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point