

N-BENZYLOXYCARBONYL-L-TYROSINE

Other names:	N-Cbz-L-tyrosine N-Carbobenzoxy-L-tyrosine L-Tyrosine, N-[(phenylmethoxy)carbonyl]-
Inchi:	InChI=1S/C17H17NO5/c19-14-8-6-12(7-9-14)10-15(16(20)21)18-17(22)23-11-13-4-2-1-3
InchiKey:	MCRMUCXATQAAMN-OAHLLOKOSA-N
Formula:	C17H17NO5
SMILES:	O=C(N[C@@H](Cc1ccc(O)cc1)C(=O)O)OCc1ccccc1
Mol. weight [g/mol]:	315.32

Physical Properties

Property code	Value	Unit	Source
hfus	43.70	kJ/mol	Joback Method
hvap	141.92	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-2.83		Cheméo Relay (1.0)
logp	2.314		Crippen Method
mcvol	233.600	ml/mol	McGowan Method
tb	657.84	K	Cheméo Relay (1.0)
tf	415.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.86	J/mol×K	994.41	Joback Method
cpg	743.33	J/mol×K	1033.67	Joback Method
cpg	753.33	J/mol×K	1072.93	Joback Method
cpg	762.97	J/mol×K	1112.19	Joback Method
cpg	772.36	J/mol×K	1151.44	Joback Method
cpg	781.63	J/mol×K	1190.70	Joback Method
cpg	790.89	J/mol×K	1229.96	Joback Method

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1164165&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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