

L-Phenylalanine, N-(2-chlorobenzoyl)-, methyl ester

Inchi:	InChI=1S/C17H16ClNO3/c1-22-17(21)15(11-12-7-3-2-4-8-12)19-16(20)13-9-5-6-10-14(1)
InchiKey:	SBBIHHYZJMQAMT-UHFFFAOYSA-N
Formula:	C17H16ClNO3
SMILES:	COC(=O)C(Cc1ccccc1)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	317.77

Physical Properties

Property code	Value	Unit	Source
hf	-368.66	kJ/mol	Cheméo Relay (1.0)
hfus	37.64	kJ/mol	Joback Method
log10ws	-4.11		Cheméo Relay (1.0)
logp	2.854		Crippen Method
mcvol	234.100	ml/mol	McGowan Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	641.40	K	Cheméo Relay (1.0)
tf	362.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.97	J/mol×K	864.02	Joback Method
cpg	674.10	J/mol×K	903.91	Joback Method
cpg	685.03	J/mol×K	943.79	Joback Method
cpg	694.83	J/mol×K	983.68	Joback Method
cpg	703.54	J/mol×K	1023.56	Joback Method
cpg	711.25	J/mol×K	1063.45	Joback Method
cpg	718.00	J/mol×K	1103.34	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299591&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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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