1,2-Propanediol, 3-(4-chlorophenoxy)-, 1-carbamate

Other names: 1,2-Propanediol, 3-(4-chlorophenoxy)-, 1-carbamate
1,2-Propanediol, 3-(p-chlorophenoxy)-, 1-carbamate
Maolate
U-19,646
3-(p-Chlorophenoxy)-2-Hydroxypropyl carbamate
3-(4-Chlorophenoxy)-2-hydroxypropyl carbamate
Carbamic acid, 3-(p-chlorophenoxy)-2-hydroxypropyl ester
Rinlaxer
U 19646
3-(p-Chlorophenoxy)-1,2-propanediol 1-carbamate
3-(4-Chlorophenoxy)-1,2-propanediol-1-carbamate
NSC 82943
Chlorphenesin

Inchi: InChI=1S/C10H12ClNO4/c11-7-1-3-9(4-2-7)15-5-8(13)6-16-10(12)14/h1-4,8,13H,5-6H2,(

InchiKey: SKPLBLUECSEIFO-UHFFFAOYSA-N

Formula: C10H12ClNO4

SMILES: NC(=O)OCC(O)COc1ccc(Cl)cc1

Mol. weight [g/mol]: 245.66

Physical Properties

Property code	Value	Unit	Source
hfus	29.24	kJ/mol	Joback Method
log10ws	-2.22		Cheméo Relay (1.0)
logp	1.175		Crippen Method
mcvol	169.400	ml/mol	McGowan Method
rinpol	1695.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1695.00		NIST Webbook
tf	343.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.89	J/mol×K	760.27	Joback Method

cpg	461.55	J/mol×K	795.58	Joback Method
cpg	470.47	J/mol×K	830.89	Joback Method
cpg	478.66	J/mol×K	866.20	Joback Method
cpg	486.12	J/mol×K	901.51	Joback Method
cpg	492.87	J/mol×K	936.83	Joback Method
cpg	498.89	J/mol×K	972.14	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C886748&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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity

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

tf: Normal melting (fusion) point