Chlorphenesin 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
CAS:	886-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-287.56	kJ/mol	Joback Method
hf	-541.15	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	83.67	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.175		Crippen Method
mcvol	169.400	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	760.27	K	Joback Method
tc	972.14	K	Joback Method
tf	494.79	K	Joback Method
vc	0.621	m3/kmol	Joback Method

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C886748&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
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
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume