Beclamide

Other names:	Propanamide, 3-chloro-N-(phenylmethyl)-
	Beclamid
	Beklamid
	N-Benzyl-«beta»-chloropropanamide
	N-Benzyl-«beta»-chloropropionamide
	N-Benzyl-3-chloropropionamide
	Chloracon
	Chlorakon
	Chloroethylphenamide
	N-(3-Chloropropionyl)benzylamine
	Hibicon
	Nidrane
	Nydran
	Nydrane
	Posedrine
	Propionamide, N-benzyl-3-chloro-
	Seclar
	Benxchlorpropamide
	Benzchlorpropamid
	Benzchlorpropamide
	Benzochlorpropamid
	Khlorakon
	Neuracen
	Posedrin
	3-Chloro-N-(phenylmethyl)propanamide
	NSC 67062
Inchi:	InChI=1S/C10H12ClNO/c11-7-6-10(13)12-8-9-4-2-1-3-5-9/h1-5H,6-8H2,(H,12,13)
InchiKey:	JPYQFYIEOUVJDU-UHFFFAOYSA-N
Formula:	C10H12ClNO
SMILES:	O=C(CCCl)NCc1ccccc1
Mol. weight [g/mol]:	197.66
CAS:	501-68-8

Physical Properties

Property code	Value	Unit	Source
gf	94.27	kJ/mol	Joback Method

hf	-88.05	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.932		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1697.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	596.35	K	Joback Method
tc	815.52	K	Joback Method
tf	361.39	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.98	J/mol×K	596.35	Joback Method
cpg	362.89	J/mol×K	632.88	Joback Method
cpg	374.91	J/mol×K	669.41	Joback Method
cpg	386.10	J/mol×K	705.94	Joback Method
cpg	396.50	J/mol×K	742.46	Joback Method
cpg	406.15	J/mol×K	778.99	Joback Method
cpg	415.08	J/mol×K	815.52	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=C501688&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