Benzoic acid, p-[n-(3-chloro-2-hydroxypropyl)acetamido]-, ethyl ester

InchI: InChI=1S/C14H18ClNO4/c1-3-20-14(19)11-4-6-12(7-5-11)16(10(2)17)9-13(18)8-15/h4-7
InchiKey: JNYXBBCQPHLTGN-UHFFFAOYSA-N
Formula: C14H18ClNO4
SMILES: CCOC(=O)c1ccc(N(CC(O)CCl)C(C)=O)cc1
Mol. weight [g/mol]: 299.75

Physical Properties

Property code	Value	Unit	Source
gf	-233.47	kJ/mol	Joback Method
hf	-570.33	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	88.32	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.816		Crippen Method
mcvol	221.460	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	823.15	K	Joback Method
tc	1027.58	K	Joback Method
tf	516.78	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.38	J/mol×K	823.15	Joback Method
cpg	643.65	J/mol×K	857.22	Joback Method
cpg	654.08	J/mol×K	891.29	Joback Method
cpg	663.69	J/mol×K	925.37	Joback Method
cpg	672.53	J/mol×K	959.44	Joback Method
cpg	680.62	J/mol×K	993.51	Joback Method
cpg	688.00	J/mol×K	1027.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=B6009946&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume