Glycine, N-(5-chlorovaleryl)-, methyl ester

Inchi: InChI=1S/C8H14ClNO3/c1-13-8(12)6-10-7(11)4-2-3-5-9/h2-6H2,1H3,(H,10,11)
InchiKey: DSJFHGNKSIAIHB-UHFFFAOYSA-N
Formula: C8H14ClNO3
SMILES: COC(=O)CNC(=O)CCCCCl
Mol. weight [g/mol]: 207.66

Physical Properties

Property code	Value	Unit	Source
gf	-268.90	kJ/mol	Joback Method
hf	-528.10	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.685		Crippen Method
mcvol	154.810	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	600.20	K	Joback Method
tc	791.11	K	Joback Method
tf	384.59	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.25	J/mol×K	600.20	Joback Method
cpg	382.50	J/mol×K	632.02	Joback Method
cpg	393.19	J/mol×K	663.84	Joback Method
cpg	403.33	J/mol×K	695.66	Joback Method
cpg	412.93	J/mol×K	727.48	Joback Method
cpg	421.99	J/mol×K	759.29	Joback Method
cpg	430.52	J/mol×K	791.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299714&Units=SI
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

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