Ethyl 5-(ethoxycarbonyloxy)pentylcarbamate

Inchi: InChI=1S/C11H21NO5/c1-3-15-10(13)12-8-6-5-7-9-17-11(14)16-4-2/h3-9H2,1-2H3,(H,12
InchiKey: ZTOALZFCZCBHPF-UHFFFAOYSA-N
Formula: C11H21NO5
SMILES: CCOC(=O)NCCCCCOC(=O)OCC
Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
gf	-441.71	kJ/mol	Joback Method
hf	-838.72	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	67.24	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.076		Crippen Method
mcvol	196.580	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
tb	676.25	K	Joback Method
tc	856.86	K	Joback Method
tf	432.94	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.84	J/mol×K	676.25	Joback Method
cpg	559.54	J/mol×K	706.35	Joback Method
cpg	572.57	J/mol×K	736.45	Joback Method
cpg	584.94	J/mol×K	766.56	Joback Method
cpg	596.63	J/mol×K	796.66	Joback Method
cpg	607.64	J/mol×K	826.76	Joback Method
cpg	617.96	J/mol×K	856.86	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=U373768&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume