Ethyl 3-(ethoxycarbonyloxy)propylcarbamate

Inchi: InChI=1S/C9H17NO5/c1-3-13-8(11)10-6-5-7-15-9(12)14-4-2/h3-7H2,1-2H3,(H,10,11)
InchiKey: LGGROSYBYDOKMR-UHFFFAOYSA-N
Formula: C9H17NO5
SMILES: CCOC(=O)NCCCOC(=O)OCC
Mol. weight [g/mol]: 219.24

Physical Properties

Property code	Value	Unit	Source
gf	-458.55	kJ/mol	Joback Method
hf	-797.44	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	62.79	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.296		Crippen Method
mcvol	168.400	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	630.49	K	Joback Method
tc	813.29	K	Joback Method
tf	410.40	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.09	J/mol×K	630.49	Joback Method
cpg	455.53	J/mol×K	660.96	Joback Method
cpg	467.42	J/mol×K	691.42	Joback Method
cpg	478.75	J/mol×K	721.89	Joback Method
cpg	489.51	J/mol×K	752.36	Joback Method
cpg	499.68	J/mol×K	782.83	Joback Method
cpg	509.26	J/mol×K	813.29	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=U373766&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

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