2-Aminopent-4-enoic acid, N-vinyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C13H21NO4/c1-4-7-8-10-18-12(15)11(9-5-2)14-13(16)17-6-3/h5-6,11H,2-4,7-1

InchiKey: CZPUGDABXVNVPJ-UHFFFAOYSA-N

Formula: C13H21NO4

SMILES: C=CCC(NC(=O)OC=C)C(=O)OCCCCC

Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
gf	-146.63	kJ/mol	Joback Method
hf	-502.20	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.534		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	692.51	K	Joback Method
tc	878.92	K	Joback Method
tf	414.73	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.64	J/mol×K	692.51	Joback Method
cpg	592.65	J/mol×K	723.58	Joback Method
cpg	605.92	J/mol×K	754.65	Joback Method
cpg	618.44	J/mol×K	785.72	Joback Method
cpg	630.22	J/mol×K	816.79	Joback Method
cpg	641.29	J/mol×K	847.86	Joback Method
cpg	651.65	J/mol×K	878.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393209&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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