2-Aminopent-4-enoic acid, N-propargyloxycarbonyl-, N-propargyl ester

Inchi: InChI=1S/C14H17NO4/c1-4-7-10-18-13(16)12(9-6-3)15-14(17)19-11-8-5-2/h1-2,6,12H,3,

InchiKey: LFIGRVKINWYBHD-UHFFFAOYSA-N

Formula: C14H17NO4

SMILES: C#CCCOC(=O)NC(CC=C)C(=O)OCCC#C

Mol. weight [g/mol]: 263.29

Physical Properties

Property code	Value	Unit	Source
gf	220.09	kJ/mol	Joback Method
hf	-64.47	kJ/mol	Joback Method
hfus	43.84	kJ/mol	Joback Method
hvap	70.16	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	1.247		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	698.95	K	Joback Method
tc	899.27	K	Joback Method
tf	521.70	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.62	J/mol×K	698.95	Joback Method
cpg	572.54	J/mol×K	732.34	Joback Method
cpg	584.69	J/mol×K	765.72	Joback Method
cpg	596.10	J/mol×K	799.11	Joback Method
cpg	606.78	J/mol×K	832.49	Joback Method
cpg	616.77	J/mol×K	865.88	Joback Method
cpg	626.07	J/mol×K	899.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393191&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