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

Inchi: InChI=1S/C17H27NO4/c1-4-7-9-10-11-14-21-16(19)15(12-6-3)18-17(20)22-13-8-5-2/h2,6

InchiKey: XICOCDSGDQZCLT-UHFFFAOYSA-N

Formula: C17H27NO4

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

Mol. weight [g/mol]: 309.40

Physical Properties

Property code	Value	Unit	Source
gf	22.28	kJ/mol	Joback Method
hf	-418.29	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.194		Crippen Method
mcvol	262.350	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	777.47	K	Joback Method
tc	967.20	K	Joback Method
tf	508.54	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.91	J/mol×K	777.47	Joback Method
cpg	789.11	J/mol×K	809.09	Joback Method
cpg	803.42	J/mol×K	840.71	Joback Method
cpg	816.86	J/mol×K	872.34	Joback Method
cpg	829.44	J/mol×K	903.96	Joback Method
cpg	841.20	J/mol×K	935.58	Joback Method
cpg	852.14	J/mol×K	967.20	Joback Method

Sources

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=U393190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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