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

Inchi: InChI=1S/C16H25NO4/c1-4-7-9-10-13-20-15(18)14(11-6-3)17-16(19)21-12-8-5-2/h2,6,14

InchiKey: REEIGQQMYFFGGM-UHFFFAOYSA-N

Formula: C16H25NO4

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

Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
gf	13.86	kJ/mol	Joback Method
hf	-397.65	kJ/mol	Joback Method
hfus	46.04	kJ/mol	Joback Method
hvap	74.76	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.804		Crippen Method
mcvol	248.260	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	754.59	K	Joback Method
tc	944.22	K	Joback Method
tf	497.27	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.42	J/mol×K	754.59	Joback Method
cpg	732.26	J/mol×K	786.19	Joback Method
cpg	746.23	J/mol×K	817.80	Joback Method
cpg	759.37	J/mol×K	849.40	Joback Method
cpg	771.69	J/mol×K	881.01	Joback Method
cpg	783.22	J/mol×K	912.61	Joback Method
cpg	793.95	J/mol×K	944.22	Joback Method

Sources

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=U393189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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