2-Aminopent-4-enoic acid, N-(but-2-yn-1-yloxycarbonyl)-, 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/h6,14H

InchiKey: NMFCXINHFGYYNW-UHFFFAOYSA-N

Formula: C16H25NO4

SMILES: C=CCC(NC(=O)OCC#CC)C(=O)OCCCCCC

Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
gf	-6.41	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.804		Crippen Method
mcvol	248.260	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	773.47	K	Joback Method
tc	969.65	K	Joback Method
tf	556.40	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.40	J/mol×K	773.47	Joback Method
cpg	736.51	J/mol×K	806.17	Joback Method
cpg	750.70	J/mol×K	838.86	Joback Method
cpg	763.98	J/mol×K	871.56	Joback Method
cpg	776.37	J/mol×K	904.26	Joback Method
cpg	787.88	J/mol×K	936.95	Joback Method
cpg	798.51	J/mol×K	969.65	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=U393193&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