1-Aminocyclopentanecarboxylic acid, N-(but-3-yn-1-yloxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C16H25NO4/c1-3-5-9-13-20-14(18)16(10-7-8-11-16)17-15(19)21-12-6-4-2/h2H

InchiKey: YSXZALIILBJIHY-UHFFFAOYSA-N

Formula: C16H25NO4

SMILES: C#CCCOC(=O)NC1(C(=O)OCCCCC)CCCC1

Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
gf	-40.48	kJ/mol	Joback Method
hf	-442.08	kJ/mol	Joback Method
hfus	38.48	kJ/mol	Joback Method
hvap	74.92	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.782		Crippen Method
mcvol	241.700	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	773.87	K	Joback Method
tc	980.93	K	Joback Method
tf	548.83	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.45	J/mol×K	773.87	Joback Method
cpg	745.30	J/mol×K	808.38	Joback Method
cpg	761.49	J/mol×K	842.89	Joback Method
cpg	777.12	J/mol×K	877.40	Joback Method
cpg	792.29	J/mol×K	911.91	Joback Method
cpg	807.11	J/mol×K	946.42	Joback Method
cpg	821.67	J/mol×K	980.93	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=U392570&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