

2-Aminopent-4-enoic acid, N-(but-2-yn-1-yloxycarbonyl)-, but-2-yn-1-yl

Inchi:
ester

InChI=1S/C14H17NO4/c1-4-7-10-18-13(16)12(9-6-3)15-14(17)19-11-8-5-2/h6,12H,3,9-1

InchiKey:

TYKGGJIMFGHDCW-UHFFFAOYSA-N

Formula:

C14H17NO4

SMILES:

C=CCC(NC(=O)OCC#CC)C(=O)OCC#CC

Mol. weight [g/mol]:

263.29

Physical Properties

Property code	Value	Unit	Source
gf	179.55	kJ/mol	Joback Method
hf	-103.67	kJ/mol	Joback Method
hfus	44.13	kJ/mol	Joback Method
hvap	74.75	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	1.247		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpola	1968.00		NIST Webbook
rinpola	1968.00		NIST Webbook
tb	736.71	K	Joback Method
tc	953.36	K	Joback Method
tf	639.96	K	Joback Method
vc	0.801	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.48	J/molxK	736.71	Joback Method
cpg	577.18	J/molxK	772.82	Joback Method
cpg	590.01	J/molxK	808.93	Joback Method
cpg	601.95	J/molxK	845.04	Joback Method
cpg	613.02	J/molxK	881.15	Joback Method
cpg	623.21	J/molxK	917.25	Joback Method
cpg	632.54	J/molxK	953.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U393198&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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