D-Alanine, N-propargyloxycarbonyl-, propargyl ester

Inchi: InChI=1S/C10H11NO4/c1-4-6-14-9(12)8(3)11-10(13)15-7-5-2/h1-2,8H,6-7H2,3H3,(H,11,

InchiKey: DUPASYGKEDEDEO-UHFFFAOYSA-N

Formula: C10H11NO4

SMILES: C#CCOC(=O)C(C)N=C(O)OCC#C

Mol. weight [g/mol]: 209.20

Physical Properties

Property code	Value	Unit	Source
hf	-128.03	kJ/mol	Joback Method
hvap	68.82	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.115		Crippen Method
mcvol	159.420	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	675.45	K	Joback Method
tc	879.99	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U347745&Units=SI

Legend

hf: Enthalpy of formation 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