1-Aminocyclopentanecarboxylic acid, N-(propargyloxycarbonyl)-, isohexyl ester

Inchi: InChI=1S/C16H25NO4/c1-4-11-21-15(19)17-16(9-5-6-10-16)14(18)20-12-7-8-13(2)3/h1,1

InchiKey: PRERIQGCXHNQOY-UHFFFAOYSA-N

Formula: C16H25NO4

SMILES: C#CCOC(=O)NC1(C(=O)OCCCC(C)C)CCCC1

Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
gf	-42.92	kJ/mol	Joback Method
hf	-447.36	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	74.53	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.638		Crippen Method
mcvol	241.700	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	773.43	K	Joback Method
tc	983.47	K	Joback Method
tf	533.83	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.98	J/mol×K	773.43	Joback Method
cpg	746.08	J/mol×K	808.44	Joback Method
cpg	762.48	J/mol×K	843.44	Joback Method
cpg	778.30	J/mol×K	878.45	Joback Method
cpg	793.64	J/mol×K	913.46	Joback Method
cpg	808.61	J/mol×K	948.47	Joback Method
cpg	823.31	J/mol×K	983.47	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=U392473&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
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