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

Inchi: InChI=1S/C17H27NO4/c1-4-7-9-10-11-14-21-16(19)15(12-6-3)18-17(20)22-13-8-5-2/h6,1

InchiKey: ULZDZHKVGJCMGT-UHFFFAOYSA-N

Formula: C17H27NO4

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

Mol. weight [g/mol]: 309.40

Physical Properties

Property code	Value	Unit	Source
gf	2.01	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	48.78	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.194		Crippen Method
mcvol	262.350	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	796.35	K	Joback Method
tc	992.27	K	Joback Method
tf	567.67	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.32	J/mol×K	796.35	Joback Method
cpg	793.75	J/mol×K	829.00	Joback Method
cpg	808.22	J/mol×K	861.66	Joback Method
cpg	821.75	J/mol×K	894.31	Joback Method
cpg	834.34	J/mol×K	926.97	Joback Method
cpg	846.02	J/mol×K	959.62	Joback Method
cpg	856.79	J/mol×K	992.27	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=U393194&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