2-Aminopent-4-enoic acid, N-(but-3-en-1-yloxycarbonyl)-, heptyl ester

Inchi: InChI=1S/C17H29NO4/c1-4-7-9-10-11-14-21-16(19)15(12-6-3)18-17(20)22-13-8-5-2/h5-

InchiKey: SJLXMVUBKVVDPA-UHFFFAOYSA-N

Formula: C17H29NO4

SMILES: C=CCCOC(=O)NC(CC=C)C(=O)OCCCCCCC

Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	-112.95	kJ/mol	Joback Method
hf	-584.76	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.747		Crippen Method
mcvol	266.650	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	784.03	K	Joback Method
tc	970.46	K	Joback Method
tf	459.81	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.25	J/mol×K	784.03	Joback Method
cpg	816.91	J/mol×K	815.10	Joback Method
cpg	831.66	J/mol×K	846.17	Joback Method
cpg	845.50	J/mol×K	877.25	Joback Method
cpg	858.47	J/mol×K	908.32	Joback Method
cpg	870.59	J/mol×K	939.39	Joback Method
cpg	881.86	J/mol×K	970.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393201&Units=SI
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

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