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

Inchi: InChI=1S/C16H27NO4/c1-4-7-9-10-13-20-15(18)14(11-6-3)17-16(19)21-12-8-5-2/h5-6,14

InchiKey: WWMJLKKYJSSJGS-UHFFFAOYSA-N

Formula: C16H27NO4

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

Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
gf	-121.37	kJ/mol	Joback Method
hf	-564.12	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.357		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	761.15	K	Joback Method
tc	946.74	K	Joback Method
tf	448.54	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.99	J/mol×K	761.15	Joback Method
cpg	759.28	J/mol×K	792.08	Joback Method
cpg	773.69	J/mol×K	823.01	Joback Method
cpg	787.25	J/mol×K	853.95	Joback Method
cpg	799.97	J/mol×K	884.88	Joback Method
cpg	811.86	J/mol×K	915.81	Joback Method
cpg	822.96	J/mol×K	946.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393200&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

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