2-Aminopent-4-enoic acid, N-hexyloxycarbonyl-, butyl ester

Inchi: InChI=1S/C16H29NO4/c1-4-7-9-10-13-21-16(19)17-14(11-6-3)15(18)20-12-8-5-2/h6,14H

InchiKey: LQEMUUPCYQBSMK-UHFFFAOYSA-N

Formula: C16H29NO4

SMILES: C=CCC(NC(=O)OCCCCCC)C(=O)OCCCC

Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
gf	-209.21	kJ/mol	Joback Method
hf	-689.55	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	74.90	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.581		Crippen Method
mcvol	256.860	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	764.47	K	Joback Method
tc	948.61	K	Joback Method
tf	450.30	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.58	J/mol×K	764.47	Joback Method
cpg	785.39	J/mol×K	795.16	Joback Method
cpg	800.31	J/mol×K	825.85	Joback Method
cpg	814.35	J/mol×K	856.54	Joback Method
cpg	827.53	J/mol×K	887.23	Joback Method
cpg	839.85	J/mol×K	917.92	Joback Method
cpg	851.34	J/mol×K	948.61	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=U393139&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