

2-Aminopent-4-enoic acid, N-(2-ethylhexyloxycarbonyl)-, dodecyl ester

Inchi: InChI=1S/C26H49NO4/c1-5-9-11-12-13-14-15-16-17-18-21-30-25(28)24(19-7-3)27-26(29)
InchiKey: QHHDXDGJFAJGOM-UHFFFAOYSA-N
Formula: C₂₆H₄₉NO₄
SMILES: C=CCC(N=C(O)OCC(CC)CCCC)C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
hf	-921.92	kJ/mol	Joback Method
hvap	103.66	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.542		Crippen Method
mcvol	397.760	ml/mol	McGowan Method
pc	756.82	kPa	Joback Method
rinpol	2863.00		NIST Webbook
rinpol	2863.00		NIST Webbook
tb	1057.53	K	Joback Method
tc	1318.34	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393167&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

hf: Enthalpy of formation 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

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