2-Aminopent-4-enoic acid, N-decyloxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C29H55NO4/c1-4-7-9-11-13-15-16-17-19-20-22-25-33-28(31)27(24-6-3)30-29(

InchiKey: YNEXQKQSBWKRJE-UHFFFAOYSA-N

Formula: C29H55NO4

SMILES: C=CCC(NC(=O)OCCCCCCCCCC)C(=O)OCCCCCCCCCCCCC

Mol. weight [g/mol]: 481.75

Physical Properties

Property code	Value	Unit	Source
gf	-99.75	kJ/mol	Joback Method
hf	-957.87	kJ/mol	Joback Method
hfus	76.74	kJ/mol	Joback Method
hvap	103.84	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	8.652		Crippen Method
mcvol	440.030	ml/mol	McGowan Method
pc	675.70	kPa	Joback Method
rinpol	3240.00		NIST Webbook
rinpol	3240.00		NIST Webbook
tb	1061.91	K	Joback Method
tc	1332.60	K	Joback Method
tf	596.81	K	Joback Method
vc	1.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1574.14	J/mol×K	1061.91	Joback Method
cpg	1596.40	J/mol×K	1107.03	Joback Method
cpg	1616.24	J/mol×K	1152.14	Joback Method
cpg	1633.80	J/mol×K	1197.26	Joback Method
cpg	1649.21	J/mol×K	1242.37	Joback Method
cpg	1662.58	J/mol×K	1287.49	Joback Method
cpg	1674.05	J/mol×K	1332.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393179&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