DL-3-Aminobutanoyl-DL-aminobutanoic acid, N-(2-ethylhexyl)oxycarbonyl-, 2-ethylhexyl ester

Inchi: InChI=1S/C25H48N2O5/c1-7-11-13-21(9-3)17-31-24(29)16-20(6)26-23(28)15-19(5)27-25(30)32-18-22(10-4)14-12-8-2/h19-22H,7-18H2,1-6H3,(H,26,28)(H,27,30)

InchiKey: BMWJKTVNOCIULN-UHFFFAOYSA-N

Formula: C25H48N2O5

SMILES: CCCCC(CC)COC(=O)CC(C)NC(=O)CC(C)NC(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-268.12	kJ/mol	Joback Method
hf	-1075.69	kJ/mol	Joback Method
hfus	63.78	kJ/mol	Joback Method
hvap	107.62	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.362		Crippen Method
mcvol	399.520	ml/mol	McGowan Method
pc	862.51	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	1076.43	K	Joback Method
tc	1334.55	K	Joback Method
tf	611.08	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.59	J/mol×K	1076.43	Joback Method
cpg	1441.33	J/mol×K	1119.45	Joback Method
cpg	1455.85	J/mol×K	1162.47	Joback Method
cpg	1468.22	J/mol×K	1205.49	Joback Method
cpg	1478.52	J/mol×K	1248.51	Joback Method
cpg	1486.84	J/mol×K	1291.53	Joback Method
cpg	1493.25	J/mol×K	1334.55	Joback Method

Sources

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=U392830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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