l-Norvaline, n-propoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C25H49NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-29-24(27)23(20-5-

InchiKey: BJPLBEWLHQKOCX-UHFFFAOYSA-N

Formula: C25H49NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCC

Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
gf	-221.27	kJ/mol	Joback Method
hf	-1000.74	kJ/mol	Joback Method
hfus	67.66	kJ/mol	Joback Method
hvap	95.60	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	7.316		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	814.00	kPa	Joback Method
tb	973.71	K	Joback Method
tc	1200.23	K	Joback Method
tf	553.49	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.27	J/mol×K	973.71	Joback Method
cpg	1367.53	J/mol×K	1011.46	Joback Method
cpg	1386.03	J/mol×K	1049.22	Joback Method
cpg	1402.82	J/mol×K	1086.97	Joback Method
cpg	1417.96	J/mol×K	1124.72	Joback Method
cpg	1431.51	J/mol×K	1162.47	Joback Method
cpg	1443.52	J/mol×K	1200.23	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=U320741&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume