l-Norvaline, n-propoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C21H41NO4/c1-4-7-8-9-10-11-12-13-14-15-18-25-20(23)19(16-5-2)22-21(24)2
InchiKey: BLWKULSJFBKTKU-UHFFFAOYSA-N
Formula: C21H41NO4
SMILES: CCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCC
Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
gf	-254.95	kJ/mol	Joback Method
hf	-918.18	kJ/mol	Joback Method
hfus	57.30	kJ/mol	Joback Method
hvap	86.70	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.755		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	882.19	K	Joback Method
tc	1080.05	K	Joback Method
tf	508.41	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.61	J/mol×K	882.19	Joback Method
cpg	1113.89	J/mol×K	915.17	Joback Method
cpg	1130.92	J/mol×K	948.14	Joback Method
cpg	1146.71	J/mol×K	981.12	Joback Method
cpg	1161.29	J/mol×K	1014.10	Joback Method
cpg	1174.70	J/mol×K	1047.07	Joback Method
cpg	1186.95	J/mol×K	1080.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320738&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