l-Norvaline, N-isobutoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C24H47NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-19-28-23(26)22(18-6-2)25-2
InchiKey: XUBKZBMNDFIXLE-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-232.13	kJ/mol	Joback Method
hf	-985.38	kJ/mol	Joback Method
hfus	61.54	kJ/mol	Joback Method
hvap	92.99	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.782		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	864.54	kPa	Joback Method
rinpol	2445.00		NIST Webbook
tb	950.39	K	Joback Method
tc	1166.86	K	Joback Method
tf	527.22	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1284.03	J/mol×K	950.39	Joback Method
cpg	1303.59	J/mol×K	986.47	Joback Method
cpg	1321.56	J/mol×K	1022.55	Joback Method
cpg	1337.96	J/mol×K	1058.63	Joback Method
cpg	1352.86	J/mol×K	1094.71	Joback Method
cpg	1366.28	J/mol×K	1130.78	Joback Method
cpg	1378.28	J/mol×K	1166.86	Joback Method

Sources

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=U320722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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