

L-Norvaline, N-propoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C13H25NO4/c1-4-7-10-17-12(15)11(8-5-2)14-13(16)18-9-6-3/h11H,4-10H2,1-3
InchiKey:	UZEKTBQHQOIHAM-UHFFFAOYSA-N
Formula:	C13H25NO4
SMILES:	CCCCOC(=O)C(CCC)NC(=O)OCCC
Mol. weight [g/mol]:	259.35

Physical Properties

Property code	Value	Unit	Source
af	0.8069		Cheméo Relay (1.0)
hf	-933.40	kJ/mol	Cheméo Relay (1.0)
hfus	36.58	kJ/mol	Joback Method
hvap	80.21	kJ/mol	Cheméo Relay (1.0)
ie	8.98	eV	Cheméo Relay (1.0)
log10ws	-3.13		Cheméo Relay (1.0)
logp	2.635		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	555.98	K	Cheméo Relay (1.0)
tc	738.10	K	Cheméo Relay (1.0)
tf	265.82	K	Cheméo Relay (1.0)
vc	0.815	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.17	J/mol×K	699.15	Joback Method
cpg	641.27	J/mol×K	729.46	Joback Method
cpg	655.61	J/mol×K	759.77	Joback Method
cpg	669.18	J/mol×K	790.08	Joback Method
cpg	681.98	J/mol×K	820.39	Joback Method
cpg	694.03	J/mol×K	850.70	Joback Method
cpg	705.33	J/mol×K	881.01	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320730&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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