

L-Norvaline, N-ethoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C12H23NO4/c1-4-7-9-17-11(14)10(8-5-2)13-12(15)16-6-3/h10H,4-9H2,1-3H3,
InchiKey:	XLGKISXNVJDRID-UHFFFAOYSA-N
Formula:	C12H23NO4
SMILES:	CCCCOC(=O)C(CCC)NC(=O)OCC
Mol. weight [g/mol]:	245.32

Physical Properties

Property code	Value	Unit	Source
af	0.7598		Cheméo Relay (1.0)
hf	-918.75	kJ/mol	Cheméo Relay (1.0)
hfus	33.99	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
log10ws	-2.83		Cheméo Relay (1.0)
logp	2.244		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1527.00		NIST Webbook
rinpol	1527.00		NIST Webbook
tb	544.07	K	Cheméo Relay (1.0)
tc	725.20	K	Cheméo Relay (1.0)
tf	269.31	K	Cheméo Relay (1.0)
vc	0.761	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.12	J/mol×K	676.27	Joback Method
cpg	586.74	J/mol×K	706.69	Joback Method
cpg	600.64	J/mol×K	737.11	Joback Method
cpg	613.82	J/mol×K	767.53	Joback Method
cpg	626.27	J/mol×K	797.95	Joback Method
cpg	638.01	J/mol×K	828.38	Joback Method
cpg	649.03	J/mol×K	858.80	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320700&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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