

L-Norvaline, N-butoxycarbonyl-, decyl ester

Inchi: InChI=1S/C20H39NO4/c1-4-7-9-10-11-12-13-14-17-24-19(22)18(15-6-3)21-20(23)25-16-5
InchiKey: GZOOGWNIMVGTHW-UHFFFAOYSA-N
Formula: C20H39NO4
SMILES: CCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCCC
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
af	1.0546		Cheméo Relay (1.0)
hf	-1069.13	kJ/mol	Cheméo Relay (1.0)
hfus	54.71	kJ/mol	Joback Method
hvap	106.02	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-5.43		Cheméo Relay (1.0)
logp	5.365		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook
tb	608.83	K	Cheméo Relay (1.0)
tc	809.00	K	Cheméo Relay (1.0)
tf	296.17	K	Cheméo Relay (1.0)
vc	1.198	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.07	J/mol×K	859.31	Joback Method
cpg	1051.93	J/mol×K	891.52	Joback Method
cpg	1068.63	J/mol×K	923.73	Joback Method
cpg	1084.17	J/mol×K	955.93	Joback Method
cpg	1098.59	J/mol×K	988.14	Joback Method
cpg	1111.90	J/mol×K	1020.35	Joback Method
cpg	1124.12	J/mol×K	1052.56	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320778&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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