L-Norvaline, N-isobutoxycarbonyl-, decyl ester

Inchi: InChI=1S/C20H39NO4/c1-5-7-8-9-10-11-12-13-15-24-19(22)18(14-6-2)21-20(23)25-16-1
InchiKey: PPUDGQDYHWNWCH-UHFFFAOYSA-N
Formula: C20H39NO4
SMILES: CCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
hf	-1085.21	kJ/mol	Cheméo Relay (1.0)
hfus	51.18	kJ/mol	Joback Method
hvap	102.12	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.48		Cheméo Relay (1.0)
logp	5.221		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
rinpol	2110.00		NIST Webbook
tb	611.48	K	Cheméo Relay (1.0)
tf	296.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.54	J/mol×K	858.87	Joback Method
cpg	1052.42	J/mol×K	891.14	Joback Method
cpg	1069.13	J/mol×K	923.40	Joback Method
cpg	1084.66	J/mol×K	955.67	Joback Method
cpg	1099.06	J/mol×K	987.93	Joback Method
cpg	1112.33	J/mol×K	1020.20	Joback Method
cpg	1124.51	J/mol×K	1052.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320720&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):	
Cheméo Relay (1.0, beta):	

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point