DL-Valine, N-methyl-N-(3-chloropropoxycarbonyl)-, decyl ester

Inchi: InChI=1S/C20H38ClNO4/c1-5-6-7-8-9-10-11-12-15-25-19(23)18(17(2)3)22(4)20(24)26-1
InchiKey: OCTHLMNAQSRLMQ-UHFFFAOYSA-N
Formula: C20H38ClNO4
SMILES: CCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl
Mol. weight [g/mol]: 391.97

Physical Properties

Property code	Value	Unit	Source
gf	-256.35	kJ/mol	Joback Method
hf	-904.50	kJ/mol	Joback Method
hfus	53.30	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.392		Crippen Method
mcvol	329.760	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	858.57	K	Joback Method
tc	1052.25	K	Joback Method
tf	491.87	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.07	J/mol×K	858.57	Joback Method
cpg	1062.63	J/mol×K	890.85	Joback Method
cpg	1079.03	J/mol×K	923.13	Joback Method
cpg	1094.29	J/mol×K	955.41	Joback Method
cpg	1108.45	J/mol×K	987.69	Joback Method
cpg	1121.53	J/mol×K	1019.97	Joback Method
cpg	1133.57	J/mol×K	1052.25	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=U392980&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

Latest version available from:
https://www.chemeo.com/cid/122-963-7/DL-Valine-N-methyl-N-3-chloropropoxycarbonyl-decyl-ester.pdf
Generated by Cheméo on 2024-05-12 08:49:55.020597325 +0000 UTC m=+17793043.941174642.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.