DL-Valine, N-methyl-N-octyloxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C19H37NO4/c1-7-8-9-10-11-12-13-23-19(22)20(6)17(16(4)5)18(21)24-14-15(2

InchiKey: JBYAJVOYFQKYEW-UHFFFAOYSA-N

Formula: C19H37NO4

SMILES: CCCCCCCCOC(=O)N(C)C(C(=O)OCC(C)C)C(C)C

Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	-255.28	kJ/mol	Joback Method
hf	-873.40	kJ/mol	Joback Method
hfus	42.99	kJ/mol	Joback Method
hvap	77.08	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.639		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	797.82	K	Joback Method
tc	982.82	K	Joback Method
tf	435.68	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.34	J/mol×K	797.82	Joback Method
cpg	971.63	J/mol×K	828.65	Joback Method
cpg	988.84	J/mol×K	859.49	Joback Method
cpg	1005.00	J/mol×K	890.32	Joback Method
cpg	1020.12	J/mol×K	921.15	Joback Method
cpg	1034.23	J/mol×K	951.99	Joback Method
cpg	1047.35	J/mol×K	982.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U392899&Units=SI

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