

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

Inchi:	InChI=1S/C24H47NO4/c1-6-8-10-12-14-16-17-19-28-23(26)22(21(3)4)25(5)24(27)29-20
InchiKey:	PQGKCSWPQSSGDY-UHFFFAOYSA-N
Formula:	C24H47NO4
SMILES:	CCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]:	413.63

Physical Properties

Property code	Value	Unit	Source
gf	-210.74	kJ/mol	Joback Method
hf	-971.32	kJ/mol	Joback Method
hfus	59.46	kJ/mol	Joback Method
hvap	88.60	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.734		Crippen Method
mvol	373.880	ml/mol	McGowan Method
pc	856.97	kPa	Joback Method
rinpol	2621.00		NIST Webbook
rinpol	2621.00		NIST Webbook
tb	912.66	K	Joback Method
tc	1118.65	K	Joback Method
tf	507.03	K	Joback Method
vc	1.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.02	J/mol×K	912.66	Joback Method
cpg	1283.26	J/mol×K	946.99	Joback Method
cpg	1302.04	J/mol×K	981.32	Joback Method
cpg	1319.40	J/mol×K	1015.66	Joback Method
cpg	1335.38	J/mol×K	1049.99	Joback Method
cpg	1350.03	J/mol×K	1084.32	Joback Method
cpg	1363.40	J/mol×K	1118.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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