

DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(but-4-en-1-yloxycarbonyl)-, heptyl ester

InChI: InChI=1S/C20H36N2O5/c1-7-9-11-12-13-15-26-19(24)17(4)21(5)18(23)16(3)22(6)20(25)
InChIKey: TXOINJUMZHFZJE-UHFFFAOYSA-N

Formula: C20H36N2O5

SMILES: C=CCCOC(=O)N(C)C(C)C(=O)N(C)C(C)C(=O)OCCCCCCC

Mol. weight [g/mol]: 384.51

Physical Properties

Property code	Value	Unit	Source
gf	-174.72	kJ/mol	Joback Method
hf	-808.38	kJ/mol	Joback Method
hfus	52.44	kJ/mol	Joback Method
hvap	87.81	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.380		Crippen Method
mcvol	324.770	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook
tb	884.13	K	Joback Method
tc	1083.09	K	Joback Method
tf	542.59	K	Joback Method
vc	1.214	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.02	J/molxK	884.13	Joback Method
cpg	1067.60	J/molxK	917.29	Joback Method
cpg	1082.98	J/molxK	950.45	Joback Method
cpg	1097.21	J/molxK	983.61	Joback Method
cpg	1110.33	J/molxK	1016.77	Joback Method
cpg	1122.37	J/molxK	1049.93	Joback Method
cpg	1133.38	J/molxK	1083.09	Joback Method

Sources

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=U392747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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