

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

Inchi: C17H28N2O5
InchiKey: AYVPGDQUTYNVPN-UHFFFAOYSA-N
Formula: C₁₇H₂₈N₂O₅
SMILES: C=CCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCC=C
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-112.14	kJ/mol	Joback Method
hf	-621.03	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.986		Crippen Method
mcvol	278.200	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	812.17	K	Joback Method
tc	1003.82	K	Joback Method
tf	507.02	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.52	J/molxK	812.17	Joback Method
cpg	860.60	J/molxK	844.11	Joback Method
cpg	874.69	J/molxK	876.05	Joback Method
cpg	887.82	J/molxK	907.99	Joback Method
cpg	900.02	J/molxK	939.94	Joback Method
cpg	911.32	J/molxK	971.88	Joback Method
cpg	921.75	J/molxK	1003.82	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=U392750&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
hvac:	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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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