

DL-Alanine, N-methyl-N-(but-4-en-1-yloxycarbonyl)-, heptyl ester

InChI: InChI=1S/C16H29NO4/c1-5-7-9-10-11-13-20-15(18)14(3)17(4)16(19)21-12-8-6-2/h6,14H
InChIKey: WWWKZUKESDFZMR-UHFFFAOYSA-N

Formula: C16H29NO4
SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCC
Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
gf	-187.82	kJ/mol	Joback Method
hf	-675.49	kJ/mol	Joback Method
hfus	40.99	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.533		Crippen Method
mcvol	256.860	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	726.74	K	Joback Method
tc	906.22	K	Joback Method
tf	430.11	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.62	J/mol×K	726.74	Joback Method
cpg	767.04	J/mol×K	756.65	Joback Method
cpg	782.60	J/mol×K	786.57	Joback Method
cpg	797.31	J/mol×K	816.48	Joback Method
cpg	811.18	J/mol×K	846.39	Joback Method
cpg	824.23	J/mol×K	876.31	Joback Method
cpg	836.48	J/mol×K	906.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392732&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
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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