

DL-Alanine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, (1R)-(-)-menthyl ester

InChI=1S/C25H45NO4/c1-15(2)20-11-10-18(6)22(14-20)29-24(27)19(7)26(8)25(28)30-23
InChIKey: FJKOLRYQWXTQSX-UHFFFAOYSA-N

Formula: C25H45NO4

SMILES: CC1CCC(C(C)C)C(OC(=O)N(C)C(C)C(=O)OC2CC(C(C)C)CCC2C)C1

Mol. weight [g/mol]: 423.63

Physical Properties

Property code	Value	Unit	Source
gf	-186.70	kJ/mol	Joback Method
hf	-969.96	kJ/mol	Joback Method
hfus	46.49	kJ/mol	Joback Method
hvap	90.06	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.908		Crippen Method
mcvol	366.250	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	955.52	K	Joback Method
tc	1175.14	K	Joback Method
tf	501.10	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.65	J/molxK	955.52	Joback Method
cpg	1356.58	J/molxK	992.12	Joback Method
cpg	1374.25	J/molxK	1028.73	Joback Method
cpg	1389.71	J/molxK	1065.33	Joback Method
cpg	1402.98	J/molxK	1101.94	Joback Method
cpg	1414.09	J/molxK	1138.54	Joback Method
cpg	1423.08	J/molxK	1175.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392806&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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