

DL-Alanine, N-methyl-N-hexyloxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C20H39NO4/c1-5-7-9-11-12-13-15-16-24-19(22)18(3)21(4)20(23)25-17-14-10
InchiKey:	BANIQTOVCTWIFD-UHFFFAOYSA-N
Formula:	C20H39NO4
SMILES:	CCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCC
Mol. weight [g/mol]:	357.53

Physical Properties

Property code	Value	Unit	Source
gf	-241.98	kJ/mol	Joback Method
hf	-883.48	kJ/mol	Joback Method
hfus	52.63	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.317		Crippen Method
mvol	317.520	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	821.58	K	Joback Method
tc	1007.58	K	Joback Method
tf	476.95	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.06	J/mol×K	821.58	Joback Method
cpg	1031.54	J/mol×K	852.58	Joback Method
cpg	1048.91	J/mol×K	883.58	Joback Method
cpg	1065.21	J/mol×K	914.58	Joback Method
cpg	1080.46	J/mol×K	945.58	Joback Method
cpg	1094.68	J/mol×K	976.58	Joback Method
cpg	1107.89	J/mol×K	1007.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392638&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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