DL-Alanine, N-methyl-N-decyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C20H39NO4/c1-5-7-9-10-11-12-13-15-17-25-20(23)21(4)18(3)19(22)24-16-14-

InchiKey: XGAWBUZRLFPQBS-UHFFFAOYSA-N

Formula: C20H39NO4

SMILES: CCCCCCCCCCOC(=O)N(C)C(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
mcvol	317.520	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
tb	821.58	K	Joback Method
tc	1007.58	K	Joback Method
tf	476.95	K	Joback Method
vc	1.216	m3/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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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