

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

Inchi: InChI=1S/C26H51NO4/c1-5-7-9-11-12-13-14-15-16-17-18-19-21-22-30-25(28)24(3)27(4)
InchiKey: MTUWNUZVRGXKRQ-UHFFFAOYSA-N
Formula: C26H51NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCC
Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
gf	-191.46	kJ/mol	Joback Method
hf	-1007.32	kJ/mol	Joback Method
hfus	68.17	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.658		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	764.79	kPa	Joback Method
rinpol	2866.00		NIST Webbook
rinpol	2866.00		NIST Webbook
tb	958.86	K	Joback Method
tc	1182.25	K	Joback Method
tf	544.57	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.62	J/mol×K	958.86	Joback Method
cpg	1412.14	J/mol×K	996.09	Joback Method
cpg	1431.93	J/mol×K	1033.32	Joback Method
cpg	1450.04	J/mol×K	1070.56	Joback Method
cpg	1466.53	J/mol×K	1107.79	Joback Method
cpg	1481.49	J/mol×K	1145.02	Joback Method
cpg	1494.96	J/mol×K	1182.25	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=U392644&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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