

DL-Alanyl-DL-alanyl-DL-alanine, N,N',N''-trimethyl-N''-octyloxycarbonyl-, octyl

Inchi:
ester

InChI=1S/C29H55N3O6/c1-9-11-13-15-17-19-21-37-28(35)25(5)31(7)26(33)23(3)30(6)2

InchiKey:

PQQDOLGKLAJPMB-UHFFFAOYSA-N

Formula:

C29H55N3O6

SMILES:

CCCCCCCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCCCCCCC

Mol. weight [g/mol]:

541.76

Physical Properties

Property code	Value	Unit	Source
gf	-207.36	kJ/mol	Joback Method
hf	-1169.90	kJ/mol	Joback Method
hfus	78.13	kJ/mol	Joback Method
hvap	116.92	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.401		Crippen Method
mvol	467.430	ml/mol	McGowan Method
pc	705.08	kPa	Joback Method
rinpol	3406.00		NIST Webbook
rinpol	3406.00		NIST Webbook
tb	1159.24	K	Joback Method
tc	1478.13	K	Joback Method
tf	713.18	K	Joback Method
vc	1.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1702.68	J/molxK	1159.24	Joback Method
cpg	1722.12	J/molxK	1212.39	Joback Method
cpg	1738.63	J/molxK	1265.54	Joback Method
cpg	1752.50	J/molxK	1318.68	Joback Method
cpg	1763.97	J/molxK	1371.83	Joback Method
cpg	1773.33	J/molxK	1424.98	Joback Method
cpg	1780.85	J/molxK	1478.13	Joback Method

Sources

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=U392658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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