D-Alanine, N-neopentyloxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C22H43NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-26-20(24)19(2)23-21(25)27-

InchiKey: AMECOOPDZSVILG-UHFFFAOYSA-N

Formula: C22H43NO4

SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)OCC(C)(C)C

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-243.69	kJ/mol	Joback Method
hf	-947.57	kJ/mol	Joback Method
hfus	52.47	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.001		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	2506.00		NIST Webbook
tb	901.84	K	Joback Method
tc	1104.13	K	Joback Method
tf	522.10	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.93	J/mol×K	901.84	Joback Method
cpg	1176.43	J/mol×K	935.55	Joback Method
cpg	1193.64	J/mol×K	969.27	Joback Method
cpg	1209.63	J/mol×K	1002.98	Joback Method
cpg	1224.43	J/mol×K	1036.70	Joback Method
cpg	1238.09	J/mol×K	1070.41	Joback Method
cpg	1250.67	J/mol×K	1104.13	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=U347771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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