D-Alanine, N-neopentyloxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C27H53NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-31-25(29)24
InchiKey: XNGKRKVGOKEXCU-UHFFFAOYSA-N
Formula: C27H53NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
gf	-201.59	kJ/mol	Joback Method
hf	-1050.77	kJ/mol	Joback Method
hfus	65.42	kJ/mol	Joback Method
hvap	98.76	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	7.952		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	739.22	kPa	Joback Method
rinpol	2980.00		NIST Webbook
rinpol	2980.00		NIST Webbook
tb	1016.24	K	Joback Method
tc	1256.74	K	Joback Method
tf	578.45	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.30	J/mol×K	1016.24	Joback Method
cpg	1496.36	J/mol×K	1056.32	Joback Method
cpg	1515.58	J/mol×K	1096.41	Joback Method
cpg	1533.07	J/mol×K	1136.49	Joback Method
cpg	1548.92	J/mol×K	1176.57	Joback Method
cpg	1563.25	J/mol×K	1216.65	Joback Method
cpg	1576.15	J/mol×K	1256.74	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=U347776&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