D-alanine, n-neopentyloxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C23H45NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-27-21(25)20(2)24-22(26)

InchiKey: AOQKGYSNHFYTQJ-UHFFFAOYSA-N

Formula: C23H45NO4

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

Mol. weight [g/mol]: 399.62

Physical Properties

Property code	Value	Unit	Source
hf	-1163.86	kJ/mol	Cheméo Relay (1.0)
hfus	55.06	kJ/mol	Joback Method
hvap	114.52	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.57		Cheméo Relay (1.0)
logp	6.391		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
rinpol	2602.00		NIST Webbook
tb	623.63	K	Cheméo Relay (1.0)
tf	344.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.46	J/mol×K	924.72	Joback Method
cpg	1239.37	J/mol×K	959.34	Joback Method
cpg	1256.92	J/mol×K	993.95	Joback Method
cpg	1273.17	J/mol×K	1028.57	Joback Method
cpg	1288.16	J/mol×K	1063.19	Joback Method
cpg	1301.96	J/mol×K	1097.80	Joback Method
cpg	1314.60	J/mol×K	1132.42	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347772&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point