

D-Alanine, N-neopentylloxycarbonyl-, 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:	CCCCCCCCCCCCCOC(=O)C(C)NC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	399.61

Physical Properties

Property code	Value	Unit	Source
gf	-235.27	kJ/mol	Joback Method
hf	-968.21	kJ/mol	Joback Method
hfus	55.06	kJ/mol	Joback Method
hvap	89.86	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.391		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	921.62	kPa	Joback Method
rinqol	2602.00		NIST Webbook
tb	924.72	K	Joback Method
tc	1132.42	K	Joback Method
tf	533.37	K	Joback Method
vc	1.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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