D-Alanine, N-ethoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C23H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-28-22(25)21(3)2

InchiKey: GWCLXJQNIJHARS-UHFFFAOYSA-N

Formula: C23H45NO4

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

Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
gf	-238.11	kJ/mol	Joback Method
hf	-959.46	kJ/mol	Joback Method
hfus	62.48	kJ/mol	Joback Method
hvap	91.15	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.536		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	911.08	kPa	Joback Method
rinpol	2721.00		NIST Webbook
rinpol	2721.00		NIST Webbook
tb	927.95	K	Joback Method
tc	1137.94	K	Joback Method
tf	530.95	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.46	J/mol×K	927.95	Joback Method
cpg	1239.66	J/mol×K	962.95	Joback Method
cpg	1257.39	J/mol×K	997.95	Joback Method
cpg	1273.68	J/mol×K	1032.94	Joback Method
cpg	1288.57	J/mol×K	1067.94	Joback Method
cpg	1302.11	J/mol×K	1102.94	Joback Method
cpg	1314.31	J/mol×K	1137.94	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=U347760&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