D-Alanine, N-butoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C20H39NO4/c1-4-6-8-9-10-11-12-13-14-15-17-24-19(22)18(3)21-20(23)25-16-
InchiKey: XORTWTIOWWCJLX-UHFFFAOYSA-N
Formula: C20H39NO4
SMILES: CCCCCCCCCCCCOC(=O)C(C)NC(=O)OCCCC
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	-263.37	kJ/mol	Joback Method
hf	-897.54	kJ/mol	Joback Method
hfus	54.71	kJ/mol	Joback Method
hvap	84.47	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.365		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2415.00		NIST Webbook
tb	859.31	K	Joback Method
tc	1052.56	K	Joback Method
tf	497.14	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.07	J/mol×K	859.31	Joback Method
cpg	1051.93	J/mol×K	891.52	Joback Method
cpg	1068.63	J/mol×K	923.73	Joback Method
cpg	1084.17	J/mol×K	955.93	Joback Method
cpg	1098.59	J/mol×K	988.14	Joback Method
cpg	1111.90	J/mol×K	1020.35	Joback Method
cpg	1124.12	J/mol×K	1052.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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