D-Alanine, N-neopentyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C19H37NO4/c1-6-7-8-9-10-11-12-13-14-23-17(21)16(2)20-18(22)24-15-19(3,4

InchiKey: XHJBKIPBZAGJJC-UHFFFAOYSA-N

Formula: C19H37NO4

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

Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	-268.95	kJ/mol	Joback Method
hf	-885.65	kJ/mol	Joback Method
hfus	44.70	kJ/mol	Joback Method
hvap	80.95	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.831		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook
tb	833.20	K	Joback Method
tc	1024.71	K	Joback Method
tf	488.29	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.04	J/mol×K	833.20	Joback Method
cpg	991.47	J/mol×K	865.12	Joback Method
cpg	1007.82	J/mol×K	897.04	Joback Method
cpg	1023.10	J/mol×K	928.95	Joback Method
cpg	1037.36	J/mol×K	960.87	Joback Method
cpg	1050.63	J/mol×K	992.79	Joback Method
cpg	1062.94	J/mol×K	1024.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347768&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

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

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