

D-Alanine, N-neopentylloxycarbonyl-, undecyl ester

Inchi:	InChI=1S/C20H39NO4/c1-6-7-8-9-10-11-12-13-14-15-24-18(22)17(2)21-19(23)25-16-20
InchiKey:	PBAGFOJDLAIJHH-UHFFFAOYSA-N
Formula:	C20H39NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)NC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	357.53

Physical Properties

Property code	Value	Unit	Source
gf	-260.53	kJ/mol	Joback Method
hf	-906.29	kJ/mol	Joback Method
hfus	47.29	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.221		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
rinqol	2310.00		NIST Webbook
tb	856.08	K	Joback Method
tc	1050.34	K	Joback Method
tf	499.56	K	Joback Method
vc	1.222	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.67	J/molxK	856.08	Joback Method
cpg	1052.43	J/molxK	888.46	Joback Method
cpg	1069.04	J/molxK	920.83	Joback Method
cpg	1084.55	J/molxK	953.21	Joback Method
cpg	1098.99	J/molxK	985.59	Joback Method
cpg	1112.39	J/molxK	1017.96	Joback Method
cpg	1124.80	J/molxK	1050.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347769&Units=SI

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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