D-Alanine, N-allyloxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C20H37NO4/c1-4-6-7-8-9-10-11-12-13-14-15-17-24-19(22)18(3)21-20(23)25-1
InchiKey: ISRDLPUYIPKCJR-UHFFFAOYSA-N
Formula: C20H37NO4
SMILES: C=CCOC(=O)NC(C)C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
gf	-175.53	kJ/mol	Joback Method
hf	-772.11	kJ/mol	Joback Method
hfus	53.43	kJ/mol	Joback Method
hvap	83.80	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.141		Crippen Method
mcvol	313.220	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2416.00		NIST Webbook
tb	855.99	K	Joback Method
tc	1049.04	K	Joback Method
tf	495.38	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.16	J/mol×K	855.99	Joback Method
cpg	1023.48	J/mol×K	888.17	Joback Method
cpg	1039.68	J/mol×K	920.34	Joback Method
cpg	1054.77	J/mol×K	952.52	Joback Method
cpg	1068.80	J/mol×K	984.69	Joback Method
cpg	1081.78	J/mol×K	1016.87	Joback Method
cpg	1093.73	J/mol×K	1049.04	Joback Method

Sources

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=U347736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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