D-Alanine, N-ethoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C13H25NO4/c1-4-6-7-8-9-10-18-12(15)11(3)14-13(16)17-5-2/h11H,4-10H2,1-3
InchiKey: MLBJUTHIZUXARJ-UHFFFAOYSA-N
Formula: C13H25NO4
SMILES: CCCCCCCOC(=O)C(C)NC(=O)OCC
Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-322.31	kJ/mol	Joback Method
hf	-753.06	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.635		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1761.00		NIST Webbook
tb	699.15	K	Joback Method
tc	881.01	K	Joback Method
tf	418.25	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.17	J/mol×K	699.15	Joback Method
cpg	641.27	J/mol×K	729.46	Joback Method
cpg	655.61	J/mol×K	759.77	Joback Method
cpg	669.18	J/mol×K	790.08	Joback Method
cpg	681.98	J/mol×K	820.39	Joback Method
cpg	694.03	J/mol×K	850.70	Joback Method
cpg	705.33	J/mol×K	881.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347750&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

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