D-Alanine, N-ethoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C12H23NO4/c1-4-6-7-8-9-17-11(14)10(3)13-12(15)16-5-2/h10H,4-9H2,1-3H3,(
InchiKey: VXMQTKSUZIKFJU-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCCCCCOC(=O)C(C)NC(=O)OCC
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
gf	-330.73	kJ/mol	Joback Method
hf	-732.42	kJ/mol	Joback Method
hfus	33.99	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.244		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1659.00		NIST Webbook
tb	676.27	K	Joback Method
tc	858.80	K	Joback Method
tf	406.98	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.12	J/mol×K	676.27	Joback Method
cpg	586.74	J/mol×K	706.69	Joback Method
cpg	600.64	J/mol×K	737.11	Joback Method
cpg	613.82	J/mol×K	767.53	Joback Method
cpg	626.27	J/mol×K	797.95	Joback Method
cpg	638.01	J/mol×K	828.38	Joback Method
cpg	649.03	J/mol×K	858.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347749&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