«beta»-Alanine, N-cyclohexylcarbonyl-, decyl ester

Inchi: InChI=1S/C20H37NO3/c1-2-3-4-5-6-7-8-12-17-24-19(22)15-16-21-20(23)18-13-10-9-11-1

InchiKey: OFAOHAXHWQMURX-UHFFFAOYSA-N

Formula: C20H37NO3

SMILES: CCCCCCCCCCOC(=O)CCNC(=O)C1CCCCC1

Mol. weight [g/mol]: 339.51

Physical Properties

Property code	Value	Unit	Source
gf	-131.48	kJ/mol	Joback Method
hf	-705.72	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.757		Crippen Method
mcvol	300.790	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2659.00		NIST Webbook
rinpol	2659.00		NIST Webbook
tb	856.88	K	Joback Method
tc	1056.53	K	Joback Method
tf	497.29	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.14	J/mol×K	856.88	Joback Method
cpg	1017.61	J/mol×K	890.16	Joback Method
cpg	1034.79	J/mol×K	923.43	Joback Method
cpg	1050.72	J/mol×K	956.71	Joback Method
cpg	1065.45	J/mol×K	989.98	Joback Method
cpg	1079.00	J/mol×K	1023.26	Joback Method
cpg	1091.42	J/mol×K	1056.53	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=U321967&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
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