Sarcosine, N-(3-cyclopentylpropionyl)-, ethyl ester

Inchi: InChI=1S/C13H23NO3/c1-3-17-13(16)10-14(2)12(15)9-8-11-6-4-5-7-11/h11H,3-10H2,1-2

InchiKey: CXMFFEVRZAQVOD-UHFFFAOYSA-N

Formula: C13H23NO3

SMILES: CCOC(=O)CN(C)C(=O)CCC1CCCC1

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-156.93	kJ/mol	Joback Method
hf	-541.02	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.978		Crippen Method
mcvol	202.160	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook
tb	654.72	K	Joback Method
tc	850.50	K	Joback Method
tf	401.73	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.70	J/mol×K	654.72	Joback Method
cpg	587.14	J/mol×K	687.35	Joback Method
cpg	603.58	J/mol×K	719.98	Joback Method
cpg	619.04	J/mol×K	752.61	Joback Method
cpg	633.57	J/mol×K	785.24	Joback Method
cpg	647.18	J/mol×K	817.87	Joback Method
cpg	659.92	J/mol×K	850.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321829&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

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