Sarcosine, N-(cyclopentylcarbonyl)-, propyl ester

Inchi: InChI=1S/C12H21NO3/c1-3-8-16-11(14)9-13(2)12(15)10-6-4-5-7-10/h10H,3-9H2,1-2H3
InchiKey: ITYUXPFUTILAEO-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: CCCOC(=O)CN(C)C(=O)C1CCCC1
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-165.35	kJ/mol	Joback Method
hf	-520.38	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.588		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1754.00		NIST Webbook
tb	631.84	K	Joback Method
tc	830.00	K	Joback Method
tf	390.46	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.46	J/mol×K	631.84	Joback Method
cpg	533.53	J/mol×K	664.87	Joback Method
cpg	549.62	J/mol×K	697.89	Joback Method
cpg	564.76	J/mol×K	730.92	Joback Method
cpg	578.97	J/mol×K	763.95	Joback Method
cpg	592.29	J/mol×K	796.97	Joback Method
cpg	604.75	J/mol×K	830.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321336&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