Sarcosine, N-(cyclopentylcarbonyl)-, octyl ester

Inchi: InChI=1S/C17H31NO3/c1-3-4-5-6-7-10-13-21-16(19)14-18(2)17(20)15-11-8-9-12-15/h15

InchiKey: QKLGLEYACVDFRN-UHFFFAOYSA-N

Formula: C17H31NO3

SMILES: CCCCCCCCOC(=O)CN(C)C(=O)C1CCCC1

Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
gf	-123.25	kJ/mol	Joback Method
hf	-623.58	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	71.64	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.539		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2257.00		NIST Webbook
tb	746.24	K	Joback Method
tc	936.47	K	Joback Method
tf	446.81	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.64	J/mol×K	746.24	Joback Method
cpg	813.10	J/mol×K	777.94	Joback Method
cpg	830.49	J/mol×K	809.65	Joback Method
cpg	846.83	J/mol×K	841.35	Joback Method
cpg	862.16	J/mol×K	873.06	Joback Method
cpg	876.53	J/mol×K	904.76	Joback Method
cpg	889.96	J/mol×K	936.47	Joback Method

Sources

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=U321339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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