Sarcosine, N-(cyclopentylcarbonyl)-, dodecyl ester

Inchi: InChI=1S/C21H39NO3/c1-3-4-5-6-7-8-9-10-11-14-17-25-20(23)18-22(2)21(24)19-15-12-
InchiKey: HGXJPHCNNPQWHV-UHFFFAOYSA-N
Formula: C21H39NO3
SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)C1CCCC1
Mol. weight [g/mol]: 353.54

Physical Properties

Property code	Value	Unit	Source
gf	-89.57	kJ/mol	Joback Method
hf	-706.14	kJ/mol	Joback Method
hfus	51.49	kJ/mol	Joback Method
hvap	80.54	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.099		Crippen Method
mcvol	314.880	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	2672.00		NIST Webbook
tb	837.76	K	Joback Method
tc	1031.09	K	Joback Method
tf	491.89	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.00	J/mol×K	837.76	Joback Method
cpg	1054.32	J/mol×K	869.98	Joback Method
cpg	1072.44	J/mol×K	902.20	Joback Method
cpg	1089.41	J/mol×K	934.42	Joback Method
cpg	1105.28	J/mol×K	966.64	Joback Method
cpg	1120.10	J/mol×K	998.86	Joback Method
cpg	1133.91	J/mol×K	1031.09	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=U321342&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