l-Serine, N,O-bis(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C20H33NO5/c1-25-20(24)17(21-18(22)12-10-15-6-2-3-7-15)14-26-19(23)13-1

InchiKey: QDCGDCHKEPOQTJ-UHFFFAOYSA-N

Formula: C20H33NO5

SMILES: COC(=O)C(COC(=O)CCC1CCCC1)NC(=O)CCC1CCCC1

Mol. weight [g/mol]: 367.48

Physical Properties

Property code	Value	Unit	Source
gf	-319.19	kJ/mol	Joback Method
hf	-889.16	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	91.73	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.128		Crippen Method
mcvol	297.370	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2878.00		NIST Webbook
tb	943.74	K	Joback Method
tc	1163.63	K	Joback Method
tf	568.87	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.45	J/mol×K	943.74	Joback Method
cpg	1051.35	J/mol×K	980.39	Joback Method
cpg	1065.72	J/mol×K	1017.04	Joback Method
cpg	1078.63	J/mol×K	1053.69	Joback Method
cpg	1090.12	J/mol×K	1090.33	Joback Method
cpg	1100.25	J/mol×K	1126.98	Joback Method
cpg	1109.08	J/mol×K	1163.63	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=U299657&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

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