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

Inchi: InChI=1S/C18H33NO3/c1-3-4-5-6-9-14-22-18(21)15-19(2)17(20)13-12-16-10-7-8-11-16/h
InchiKey: AWBRZDIJHAIONR-UHFFFAOYSA-N
Formula: C18H33NO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)CCC1CCCC1
Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
gf	-114.83	kJ/mol	Joback Method
hf	-644.22	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.929		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2377.00		NIST Webbook
rinpol	2377.00		NIST Webbook
tb	769.12	K	Joback Method
tc	959.18	K	Joback Method
tf	458.08	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.47	J/mol×K	769.12	Joback Method
cpg	872.13	J/mol×K	800.80	Joback Method
cpg	889.69	J/mol×K	832.47	Joback Method
cpg	906.19	J/mol×K	864.15	Joback Method
cpg	921.67	J/mol×K	895.83	Joback Method
cpg	936.16	J/mol×K	927.51	Joback Method
cpg	949.71	J/mol×K	959.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321836&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