Sarcosine, N-(cyclohexylcarbonyl)-, octyl ester

Inchi: InChI=1S/C18H33NO3/c1-3-4-5-6-7-11-14-22-17(20)15-19(2)18(21)16-12-9-8-10-13-16/h
InchiKey: ZAGRALKGNKAAQY-UHFFFAOYSA-N
Formula: C18H33NO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)C1CCCCC1
Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
gf	-126.93	kJ/mol	Joback Method
hf	-650.38	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	74.04	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.929		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	773.39	K	Joback Method
tc	967.23	K	Joback Method
tf	454.56	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.42	J/mol×K	773.39	Joback Method
cpg	876.55	J/mol×K	805.70	Joback Method
cpg	894.47	J/mol×K	838.00	Joback Method
cpg	911.24	J/mol×K	870.31	Joback Method
cpg	926.88	J/mol×K	902.62	Joback Method
cpg	941.44	J/mol×K	934.92	Joback Method
cpg	954.95	J/mol×K	967.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321534&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