Sarcosine, N-valeryl-, octadecyl ester

Inchi: InChI=1S/C26H51NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-30-26(29)24
InchiKey: JDNKTTRHLDZIPX-UHFFFAOYSA-N
Formula: C26H51NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]: 425.69

Physical Properties

Property code	Value	Unit	Source
gf	-84.02	kJ/mol	Joback Method
hf	-869.82	kJ/mol	Joback Method
hfus	70.50	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.440		Crippen Method
mcvol	396.190	ml/mol	McGowan Method
pc	768.61	kPa	Joback Method
tb	936.88	K	Joback Method
tc	1153.23	K	Joback Method
tf	537.34	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1357.77	J/mol×K	936.88	Joback Method
cpg	1379.76	J/mol×K	972.94	Joback Method
cpg	1400.23	J/mol×K	1009.00	Joback Method
cpg	1419.24	J/mol×K	1045.05	Joback Method
cpg	1436.86	J/mol×K	1081.11	Joback Method
cpg	1453.18	J/mol×K	1117.17	Joback Method
cpg	1468.27	J/mol×K	1153.23	Joback Method

Sources

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=U321571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume