Sarcosine, N-valeryl-, heptadecyl ester

Inchi: InChI=1S/C25H49NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-22-29-25(28)23-26(3)24(27)21-5-2
InchiKey: RKAAXXKJRLMTRO-UHFFFAOYSA-N
Formula: C25H49NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]: 411.66

Physical Properties

Property code	Value	Unit	Source
gf	-92.44	kJ/mol	Joback Method
hf	-849.18	kJ/mol	Joback Method
hfus	67.91	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	7.050		Crippen Method
mcvol	382.100	ml/mol	McGowan Method
pc	811.22	kPa	Joback Method
rinpol	3120.00		NIST Webbook
rinpol	3120.00		NIST Webbook
tb	914.00	K	Joback Method
tc	1122.09	K	Joback Method
tf	526.07	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1293.43	J/mol×K	914.00	Joback Method
cpg	1314.73	J/mol×K	948.68	Joback Method
cpg	1334.61	J/mol×K	983.36	Joback Method
cpg	1353.15	J/mol×K	1018.05	Joback Method
cpg	1370.40	J/mol×K	1052.73	Joback Method
cpg	1386.43	J/mol×K	1087.41	Joback Method
cpg	1401.30	J/mol×K	1122.09	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321570&Units=SI

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