

Sarcosine, N-valeryl-, hexadecyl ester

Inchi:	InChI=1S/C24H47NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-21-28-24(27)22-25(3)
InchiKey:	GYHORPZPBPMFL-UHFFFAOYSA-N
Formula:	C24H47NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]:	397.63

Physical Properties

Property code	Value	Unit	Source
gf	-100.86	kJ/mol	Joback Method
hf	-828.54	kJ/mol	Joback Method
hfus	65.32	kJ/mol	Joback Method
hvap	86.96	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	6.659		Crippen Method
mcvol	368.010	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinsol	2966.00		NIST Webbook
tb	891.12	K	Joback Method
tc	1092.07	K	Joback Method
tf	514.80	K	Joback Method
vc	1.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1229.61	J/mol×K	891.12	Joback Method
cpg	1250.27	J/mol×K	924.61	Joback Method
cpg	1269.63	J/mol×K	958.10	Joback Method
cpg	1287.73	J/mol×K	991.60	Joback Method
cpg	1304.63	J/mol×K	1025.09	Joback Method
cpg	1320.38	J/mol×K	1058.58	Joback Method
cpg	1335.04	J/mol×K	1092.07	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=U321569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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