Sarcosine, N-(3-methylbut-2-enoyl)-, hexadecyl ester

Inchi: InChI=1S/C24H45NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-28-24(27)21-25(4)2

InchiKey: IDGQHSSDAHWMDH-UHFFFAOYSA-N

Formula: C24H45NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C=C(C)C

Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
gf	-29.19	kJ/mol	Joback Method
hf	-721.11	kJ/mol	Joback Method
hfus	64.22	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.436		Crippen Method
mcvol	363.710	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
rinpol	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook
tb	895.16	K	Joback Method
tc	1096.08	K	Joback Method
tf	495.76	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.43	J/mol×K	895.16	Joback Method
cpg	1222.45	J/mol×K	928.65	Joback Method
cpg	1241.28	J/mol×K	962.13	Joback Method
cpg	1258.99	J/mol×K	995.62	Joback Method
cpg	1275.64	J/mol×K	1029.11	Joback Method
cpg	1291.30	J/mol×K	1062.59	Joback Method
cpg	1306.03	J/mol×K	1096.08	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=U321526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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