«beta»-Alanine, N-(3-methylbut-2-enoyl)-, octadecyl ester

Inchi: InChI=1S/C26H49NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-30-26(29)20-2
InchiKey: CKIGYGSVBKQUHL-UHFFFAOYSA-N
Formula: C26H49NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCN=C(O)C=C(C)C
Mol. weight [g/mol]: 423.67

Physical Properties

Property code	Value	Unit	Source
hf	-797.14	kJ/mol	Joback Method
hvap	102.74	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	8.104		Crippen Method
mcvol	391.890	ml/mol	McGowan Method
pc	763.52	kPa	Joback Method
tb	1043.35	K	Joback Method
tc	1296.42	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321959&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

hf: Enthalpy of formation 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

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