

«beta»-Alanine, N-isobutyryl-, heptadecyl ester

Inchi:	InChI=1S/C24H47NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-28-23(26)19-20-2
InchiKey:	NELRJOGAGJVQSI-UHFFFAOYSA-N
Formula:	C24H47NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCN=C(O)C(C)C
Mol. weight [g/mol]:	397.63

Physical Properties

Property code	Value	Unit	Source
hf	-868.57	kJ/mol	Joback Method
hvac	97.86	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.404		Crippen Method
mccvol	368.010	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	993.11	K	Joback Method
tc	1226.06	K	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=U321674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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

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