

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

Inchi:	InChI=1S/C26H51NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-30-26(29)22-23
InchiKey:	JJJRVLCYDKJNHJ-UHFFFAOYSA-N
Formula:	C26H51NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]:	425.69

Physical Properties

Property code	Value	Unit	Source
gf	-105.41	kJ/mol	Joback Method
hf	-883.88	kJ/mol	Joback Method
hfus	72.58	kJ/mol	Joback Method
hvap	95.81	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.488		Crippen Method
mcvol	396.190	ml/mol	McGowan Method
pc	775.05	kPa	Joback Method
tb	974.61	K	Joback Method
tc	1203.54	K	Joback Method
tf	557.53	K	Joback Method
vc	1.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.61	J/molxK	974.61	Joback Method
cpg	1401.13	J/molxK	1012.77	Joback Method
cpg	1420.99	J/molxK	1050.92	Joback Method
cpg	1439.25	J/molxK	1089.08	Joback Method
cpg	1455.99	J/molxK	1127.23	Joback Method
cpg	1471.30	J/molxK	1165.39	Joback Method
cpg	1485.26	J/molxK	1203.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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