

«beta»-Alanine, N-(1-naphthoyl)-, nonyl ester

Inchi:	InChI=1S/C23H31NO3/c1-2-3-4-5-6-7-10-18-27-22(25)16-17-24-23(26)21-15-11-13-19-1
InchiKey:	VJWFUCNLQDHAMZ-UHFFFAOYSA-N
Formula:	C23H31NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	369.50

Physical Properties

Property code	Value	Unit	Source
gf	78.76	kJ/mol	Joback Method
hf	-405.83	kJ/mol	Joback Method
hfus	55.48	kJ/mol	Joback Method
hvap	93.71	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.254		Crippen Method
mcvol	310.700	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
tb	956.61	K	Joback Method
tc	1175.80	K	Joback Method
tf	595.36	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.24	J/molxK	956.61	Joback Method
cpg	1024.29	J/molxK	993.14	Joback Method
cpg	1038.31	J/molxK	1029.67	Joback Method
cpg	1051.37	J/molxK	1066.21	Joback Method
cpg	1063.56	J/molxK	1102.74	Joback Method
cpg	1074.96	J/molxK	1139.27	Joback Method
cpg	1085.65	J/molxK	1175.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321951&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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