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

Inchi: InChI=1S/C20H25NO3/c1-2-3-4-7-15-24-19(22)13-14-21-20(23)18-12-8-10-16-9-5-6-11-
InchiKey: SCQLMOUMBMYAIB-UHFFFAOYSA-N
Formula: C20H25NO3
SMILES: CCCCCCOC(=O)CCNC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 327.42

Physical Properties

Property code	Value	Unit	Source
gf	53.50	kJ/mol	Joback Method
hf	-343.91	kJ/mol	Joback Method
hfus	47.71	kJ/mol	Joback Method
hvap	87.03	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.083		Crippen Method
mcvol	268.430	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		NIST Webbook
tb	887.97	K	Joback Method
tc	1104.54	K	Joback Method
tf	561.55	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.20	J/mol×K	887.97	Joback Method
cpg	845.44	J/mol×K	924.07	Joback Method
cpg	858.68	J/mol×K	960.16	Joback Method
cpg	871.00	J/mol×K	996.26	Joback Method
cpg	882.46	J/mol×K	1032.35	Joback Method
cpg	893.12	J/mol×K	1068.45	Joback Method
cpg	903.07	J/mol×K	1104.54	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321948&Units=SI

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