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

Inchi: InChI=1S/C18H21NO3/c1-2-3-13-22-17(20)11-12-19-18(21)16-10-6-8-14-7-4-5-9-15(14)
InchiKey: LVBYLFSDSDOGMR-UHFFFAOYSA-N
Formula: C18H21NO3
SMILES: CCCCOC(=O)CCNC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 299.36

Physical Properties

Property code	Value	Unit	Source
gf	36.66	kJ/mol	Joback Method
hf	-302.63	kJ/mol	Joback Method
hfus	42.53	kJ/mol	Joback Method
hvap	82.58	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.303		Crippen Method
mcvol	240.250	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	2647.00		NIST Webbook
tb	842.21	K	Joback Method
tc	1060.83	K	Joback Method
tf	539.01	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.35	J/mol×K	842.21	Joback Method
cpg	730.08	J/mol×K	878.65	Joback Method
cpg	742.81	J/mol×K	915.08	Joback Method
cpg	754.63	J/mol×K	951.52	Joback Method
cpg	765.60	J/mol×K	987.96	Joback Method
cpg	775.77	J/mol×K	1024.40	Joback Method
cpg	785.22	J/mol×K	1060.83	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=U321946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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