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

Inchi: InChI=1S/C17H19NO3/c1-2-12-21-16(19)10-11-18-17(20)15-9-5-7-13-6-3-4-8-14(13)15/h
InchiKey: UTPVWDZEULQEGA-UHFFFAOYSA-N
Formula: C17H19NO3
SMILES: CCCOC(=O)CCNC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 285.34

Physical Properties

Property code	Value	Unit	Source
gf	28.24	kJ/mol	Joback Method
hf	-281.99	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	2.913		Crippen Method
mcvol	226.160	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	2547.00		NIST Webbook
rinpol	2547.00		NIST Webbook
tb	819.33	K	Joback Method
tc	1039.97	K	Joback Method
tf	527.74	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.25	J/mol×K	819.33	Joback Method
cpg	673.69	J/mol×K	856.10	Joback Method
cpg	686.15	J/mol×K	892.88	Joback Method
cpg	697.69	J/mol×K	929.65	Joback Method
cpg	708.38	J/mol×K	966.42	Joback Method
cpg	718.29	J/mol×K	1003.20	Joback Method
cpg	727.46	J/mol×K	1039.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321945&Units=SI
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

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