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

Inchi: InChI=1S/C21H27NO3/c1-2-3-4-5-8-16-25-20(23)14-15-22-21(24)19-13-9-11-17-10-6-7-
InchiKey: SMCFODOPVVAIOF-UHFFFAOYSA-N
Formula: C21H27NO3
SMILES: CCCCCCCOC(=O)CCNC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 341.44

Physical Properties

Property code	Value	Unit	Source
gf	61.92	kJ/mol	Joback Method
hf	-364.55	kJ/mol	Joback Method
hfus	50.30	kJ/mol	Joback Method
hvap	89.26	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.473		Crippen Method
mcvol	282.520	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	3036.00		NIST Webbook
tb	910.85	K	Joback Method
tc	1127.49	K	Joback Method
tf	572.82	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.83	J/mol×K	910.85	Joback Method
cpg	904.33	J/mol×K	946.96	Joback Method
cpg	917.82	J/mol×K	983.06	Joback Method
cpg	930.37	J/mol×K	1019.17	Joback Method
cpg	942.06	J/mol×K	1055.28	Joback Method
cpg	952.97	J/mol×K	1091.38	Joback Method
cpg	963.15	J/mol×K	1127.49	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=U321949&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