Sarcosine, N-(1-naphthoyl)-, isohexyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	72.45	kJ/mol	Joback Method
hf	-335.13	kJ/mol	Joback Method
hfus	42.11	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.891		Crippen Method
mcvol	268.430	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	849.80	K	Joback Method
tc	1065.30	K	Joback Method
tf	526.36	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.07	J/mol×K	849.80	Joback Method
cpg	832.25	J/mol×K	885.72	Joback Method
cpg	846.37	J/mol×K	921.63	Joback Method
cpg	859.52	J/mol×K	957.55	Joback Method
cpg	871.77	J/mol×K	993.47	Joback Method
cpg	883.19	J/mol×K	1029.39	Joback Method
cpg	893.86	J/mol×K	1065.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321403&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