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

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

Physical Properties

Property code	Value	Unit	Source
gf	74.89	kJ/mol	Joback Method
hf	-329.85	kJ/mol	Joback Method
hfus	45.63	kJ/mol	Joback Method
hvap	82.64	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.035		Crippen Method
mcvol	268.430	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	2721.00		NIST Webbook
rinpol	2721.00		NIST Webbook
tb	850.24	K	Joback Method
tc	1063.24	K	Joback Method
tf	541.36	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.53	J/mol×K	850.24	Joback Method
cpg	831.55	J/mol×K	885.74	Joback Method
cpg	845.56	J/mol×K	921.24	Joback Method
cpg	858.62	J/mol×K	956.74	Joback Method
cpg	870.81	J/mol×K	992.24	Joback Method
cpg	882.20	J/mol×K	1027.74	Joback Method
cpg	892.87	J/mol×K	1063.24	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=U321404&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