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

Inchi: InChI=1S/C21H27NO3/c1-3-4-5-6-9-15-25-20(23)16-22(2)21(24)19-14-10-12-17-11-7-8-
InchiKey: ICVCDYFXAFSJKS-UHFFFAOYSA-N
Formula: C21H27NO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 341.44

Physical Properties

Property code	Value	Unit	Source
gf	83.31	kJ/mol	Joback Method
hf	-350.49	kJ/mol	Joback Method
hfus	48.22	kJ/mol	Joback Method
hvap	84.86	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.425		Crippen Method
mcvol	282.520	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	873.12	K	Joback Method
tc	1085.62	K	Joback Method
tf	552.63	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.82	J/mol×K	873.12	Joback Method
cpg	890.08	J/mol×K	908.54	Joback Method
cpg	904.32	J/mol×K	943.95	Joback Method
cpg	917.62	J/mol×K	979.37	Joback Method
cpg	930.04	J/mol×K	1014.78	Joback Method
cpg	941.68	J/mol×K	1050.20	Joback Method
cpg	952.59	J/mol×K	1085.62	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=U321405&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