

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

Inchi:	InChI=1S/C22H29NO3/c1-3-4-5-6-7-10-16-26-21(24)17-23(2)22(25)20-15-11-13-18-12-8
InchiKey:	KBJDHTURUVJWCB-UHFFFAOYSA-N
Formula:	C22H29NO3
SMILES:	CCCCCCCCOC(=O)CN(C)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	355.47

Physical Properties

Property code	Value	Unit	Source
gf	91.73	kJ/mol	Joback Method
hf	-371.13	kJ/mol	Joback Method
hfus	50.81	kJ/mol	Joback Method
hvap	87.09	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.816		Crippen Method
mcvol	296.610	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinsol	2989.00		NIST Webbook
tb	896.00	K	Joback Method
tc	1108.72	K	Joback Method
tf	563.90	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.90	J/mol×K	896.00	Joback Method
cpg	949.41	J/mol×K	931.45	Joback Method
cpg	963.89	J/mol×K	966.91	Joback Method
cpg	977.42	J/mol×K	1002.36	Joback Method
cpg	990.09	J/mol×K	1037.81	Joback Method
cpg	1001.96	J/mol×K	1073.27	Joback Method
cpg	1013.13	J/mol×K	1108.72	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=U321406&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
mccvol:	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

Latest version available from:

<https://www.chemeo.com/cid/10-484-3/Sarcosine-N-1-naphthoyl-octyl-ester.pdf>

Generated by Cheméo on 2024-04-19 19:13:11.121521464 +0000 UTC m=+15843240.042098777.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.