

Sarcosine, N-(4-nitrobenzoyl)-, decyl ester

Inchi:	InChI=1S/C20H30N2O5/c1-3-4-5-6-7-8-9-10-15-27-19(23)16-21(2)20(24)17-11-13-18(14)
InchiKey:	ZRYFBTYJNRWBCR-UHFFFAOYSA-N
Formula:	C20H30N2O5
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	378.46

Physical Properties

Property code	Value	Unit	Source
gf	3.79	kJ/mol	Joback Method
hf	-531.68	kJ/mol	Joback Method
hfus	59.98	kJ/mol	Joback Method
hvap	97.59	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.351		Crippen Method
mcvol	305.310	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
tb	983.10	K	Joback Method
tc	1207.36	K	Joback Method
tf	652.27	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.12	J/molxK	983.10	Joback Method
cpg	1017.63	J/molxK	1020.48	Joback Method
cpg	1029.95	J/molxK	1057.85	Joback Method
cpg	1041.15	J/molxK	1095.23	Joback Method
cpg	1051.31	J/molxK	1132.61	Joback Method
cpg	1060.49	J/molxK	1169.98	Joback Method
cpg	1068.75	J/molxK	1207.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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/117-336-9/Sarcosine-N-4-nitrobenzoyl-decyl-ester.pdf>

Generated by Cheméo on 2024-05-01 03:12:13.787550114 +0000 UTC m=+16822382.708127425.

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