

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

Inchi:	InChI=1S/C21H32N2O5/c1-3-4-5-6-7-8-9-10-11-16-28-20(24)17-22(2)21(25)18-12-14-19
InchiKey:	VXMKSVJQGXRFRY-UHFFFAOYSA-N
Formula:	C21H32N2O5
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	392.49

Physical Properties

Property code	Value	Unit	Source
gf	12.21	kJ/mol	Joback Method
hf	-552.32	kJ/mol	Joback Method
hfus	62.57	kJ/mol	Joback Method
hvap	99.81	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.741		Crippen Method
mvol	319.400	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
tb	1005.98	K	Joback Method
tc	1233.11	K	Joback Method
tf	663.54	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.25	J/mol×K	1005.98	Joback Method
cpg	1077.98	J/mol×K	1043.83	Joback Method
cpg	1090.48	J/mol×K	1081.69	Joback Method
cpg	1101.84	J/mol×K	1119.54	Joback Method
cpg	1112.13	J/mol×K	1157.40	Joback Method
cpg	1121.41	J/mol×K	1195.25	Joback Method
cpg	1129.77	J/mol×K	1233.11	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321290&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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