

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

Inchi:	InChI=1S/C22H34N2O5/c1-3-4-5-6-7-8-9-10-11-12-17-29-21(25)18-23(2)22(26)19-13-15
InchiKey:	BLMNBZPEUDUOAT-UHFFFAOYSA-N
Formula:	C22H34N2O5
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	406.52

Physical Properties

Property code	Value	Unit	Source
gf	20.63	kJ/mol	Joback Method
hf	-572.96	kJ/mol	Joback Method
hfus	65.16	kJ/mol	Joback Method
hvap	102.04	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.131		Crippen Method
mcvol	333.490	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
tb	1028.86	K	Joback Method
tc	1259.86	K	Joback Method
tf	674.81	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.91	J/molxK	1028.86	Joback Method
cpg	1138.87	J/molxK	1067.36	Joback Method
cpg	1151.58	J/molxK	1105.86	Joback Method
cpg	1163.10	J/molxK	1144.36	Joback Method
cpg	1173.52	J/molxK	1182.86	Joback Method
cpg	1182.92	J/molxK	1221.36	Joback Method
cpg	1191.38	J/molxK	1259.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321291&Units=SI
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

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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