

Sarcosine, N-(4-chlorobenzoyl)-, nonyl ester

Inchi:	InChI=1S/C19H28ClNO3/c1-3-4-5-6-7-8-9-14-24-18(22)15-21(2)19(23)16-10-12-17(20)1
InchiKey:	VNSOENDCYXSYBU-UHFFFAOYSA-N
Formula:	C19H28ClNO3
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	353.88

Physical Properties

Property code	Value	Unit	Source
gf	-52.11	kJ/mol	Joback Method
hf	-516.02	kJ/mol	Joback Method
hfus	50.22	kJ/mol	Joback Method
hvap	83.16	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.706		Crippen Method
mvol	286.040	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook
tb	845.81	K	Joback Method
tc	1049.03	K	Joback Method
tf	527.31	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.66	J/mol×K	845.81	Joback Method
cpg	874.90	J/mol×K	879.68	Joback Method
cpg	889.09	J/mol×K	913.55	Joback Method
cpg	902.27	J/mol×K	947.42	Joback Method
cpg	914.48	J/mol×K	981.29	Joback Method
cpg	925.77	J/mol×K	1015.16	Joback Method
cpg	936.18	J/mol×K	1049.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U321355&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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