Sarcosine, N-(2-methoxybenzoyl)-, nonyl ester

Inchi: InChI=1S/C20H31NO4/c1-4-5-6-7-8-9-12-15-25-19(22)16-21(2)20(23)17-13-10-11-14-18
InchiKey: CESMTXWUEDTEAM-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1OC
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
gf	-136.76	kJ/mol	Joback Method
hf	-653.14	kJ/mol	Joback Method
hfus	49.80	kJ/mol	Joback Method
hvap	83.41	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.061		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2658.00		NIST Webbook
tb	853.68	K	Joback Method
tc	1053.86	K	Joback Method
tf	530.89	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.18	J/mol×K	853.68	Joback Method
cpg	936.33	J/mol×K	887.04	Joback Method
cpg	951.33	J/mol×K	920.41	Joback Method
cpg	965.21	J/mol×K	953.77	Joback Method
cpg	978.00	J/mol×K	987.13	Joback Method
cpg	989.73	J/mol×K	1020.50	Joback Method
cpg	1000.44	J/mol×K	1053.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321147&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
mcvol:	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