

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

Inchi:	InChI=1S/C20H31NO3/c1-4-5-6-7-8-9-12-15-24-19(22)16-21(3)20(23)18-14-11-10-13-17
InchiKey:	FGMOXRNATFAKDX-UHFFFAOYSA-N
Formula:	C20H31NO3
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1C
Mol. weight [g/mol]:	333.46

Physical Properties

Property code	Value	Unit	Source
gf	-31.76	kJ/mol	Joback Method
hf	-520.92	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	81.00	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.361		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2539.00		NIST Webbook
tb	831.26	K	Joback Method
tc	1030.06	K	Joback Method
tf	508.66	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.48	J/molxK	831.26	Joback Method
cpg	907.08	J/molxK	864.39	Joback Method
cpg	922.59	J/molxK	897.53	Joback Method
cpg	937.06	J/molxK	930.66	Joback Method
cpg	950.53	J/molxK	963.79	Joback Method
cpg	963.03	J/molxK	996.92	Joback Method
cpg	974.62	J/molxK	1030.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321170&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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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