

Sarcosine, N-(4-methoxybenzoyl)-, decyl ester

Inchi:	InChI=1S/C21H33NO4/c1-4-5-6-7-8-9-10-11-16-26-20(23)17-22(2)21(24)18-12-14-19(25)
InchiKey:	MTADRDQXZALRTJ-UHFFFAOYSA-N
Formula:	C21H33NO4
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	363.49

Physical Properties

Property code	Value	Unit	Source
gf	-128.34	kJ/mol	Joback Method
hf	-673.78	kJ/mol	Joback Method
hfus	52.39	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.451		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpola	2922.00		NIST Webbook
tb	876.56	K	Joback Method
tc	1078.45	K	Joback Method
tf	542.16	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.96	J/mol×K	876.56	Joback Method
cpg	996.33	J/mol×K	910.21	Joback Method
cpg	1011.50	J/mol×K	943.86	Joback Method
cpg	1025.51	J/mol×K	977.50	Joback Method
cpg	1038.38	J/mol×K	1011.15	Joback Method
cpg	1050.17	J/mol×K	1044.80	Joback Method
cpg	1060.89	J/mol×K	1078.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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