

Sarcosine, N-(3-methoxybenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C25H41NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-30-24(27)21-26(2)25(28)22
InchiKey:	ZSTDRAWJVNHKCM-UHFFFAOYSA-N
Formula:	C25H41NO4
SMILES:	CCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	419.60

Physical Properties

Property code	Value	Unit	Source
gf	-94.66	kJ/mol	Joback Method
hf	-756.34	kJ/mol	Joback Method
hfus	62.75	kJ/mol	Joback Method
hvap	94.54	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.011		Crippen Method
mvol	364.210	ml/mol	McGowan Method
pc	969.28	kPa	Joback Method
tb	968.08	K	Joback Method
tc	1185.42	K	Joback Method
tf	587.24	K	Joback Method
vc	1.393	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.19	J/mol×K	968.08	Joback Method
cpg	1242.59	J/mol×K	1004.30	Joback Method
cpg	1258.52	J/mol×K	1040.53	Joback Method
cpg	1273.04	J/mol×K	1076.75	Joback Method
cpg	1286.19	J/mol×K	1112.97	Joback Method
cpg	1298.04	J/mol×K	1149.20	Joback Method
cpg	1308.64	J/mol×K	1185.42	Joback Method

Sources

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=U321501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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