

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

Inchi:

lnchl=1S/C23H37NO3/c1-4-5-6-7-8-9-10-11-12-15-18-27-22(25)19-24(3)23(26)21-17-14

InchiKey:

MOUWNRCTRCLAMT-UHFFFAOYSA-N

Formula:

C23H37NO3

SMILES:

CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1C

Mol. weight [g/mol]:

375.54

Physical Properties

Property code	Value	Unit	Source
gf	-6.50	kJ/mol	Joback Method
hf	-582.84	kJ/mol	Joback Method
hfus	56.38	kJ/mol	Joback Method
hvap	87.67	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.531		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	899.90	K	Joback Method
tc	1104.15	K	Joback Method
tf	542.47	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1071.26	J/mol×K	899.90	Joback Method
cpg	1088.62	J/mol×K	933.94	Joback Method
cpg	1104.77	J/mol×K	967.98	Joback Method
cpg	1119.78	J/mol×K	1002.02	Joback Method
cpg	1133.70	J/mol×K	1036.07	Joback Method
cpg	1146.58	J/mol×K	1070.11	Joback Method
cpg	1158.47	J/mol×K	1104.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321173&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
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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