

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

Inchi:

YCBHFKFYRAHRBE-UHFFFAOYSA-N

InchiKey:

C15H21NO4

Formula:

CCCCOC(=O)CN(C)C(=O)c1cccc(OC)c1

SMILES:

279.33

Mol. weight [g/mol]:

Physical Properties

Property code	Value	Unit	Source
gf	-178.86	kJ/mol	Joback Method
hf	-549.94	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.110		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2224.00		NIST Webbook
tb	739.28	K	Joback Method
tc	941.06	K	Joback Method
tf	474.54	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.65	J/mol×K	739.28	Joback Method
cpg	648.56	J/mol×K	772.91	Joback Method
cpg	662.50	J/mol×K	806.54	Joback Method
cpg	675.48	J/mol×K	840.17	Joback Method
cpg	687.53	J/mol×K	873.80	Joback Method
cpg	698.66	J/mol×K	907.43	Joback Method
cpg	708.89	J/mol×K	941.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U321492&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
hvac:	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

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