

Sarcosine, n-(4-methoxybenzoyl)-, propyl ester

Inchi: InChI=1S/C14H19NO4/c1-4-9-19-13(16)10-15(2)14(17)11-5-7-12(18-3)8-6-11/h5-8H,4,9
InchiKey: QISXWZDVNHNMQB-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCCOC(=O)CN(C)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
hf	-609.06	kJ/mol	Cheméo Relay (1.0)
hfus	34.26	kJ/mol	Joback Method
hvap	86.11	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-2.65		Cheméo Relay (1.0)
logp	1.720		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
tb	620.51	K	Cheméo Relay (1.0)
tf	328.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.34	J/mol×K	716.40	Joback Method
cpg	593.90	J/mol×K	750.36	Joback Method
cpg	607.52	J/mol×K	784.33	Joback Method
cpg	620.22	J/mol×K	818.29	Joback Method
cpg	632.01	J/mol×K	852.25	Joback Method
cpg	642.91	J/mol×K	886.21	Joback Method
cpg	652.92	J/mol×K	920.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321420&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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