Sarcosine, N-(4-methylbenzoyl)-, propyl ester

Inchi: InChI=1S/C14H19NO3/c1-4-9-18-13(16)10-15(3)14(17)12-7-5-11(2)6-8-12/h5-8H,4,9-10
InchiKey: GMFAKFRABWWYLH-UHFFFAOYSA-N
Formula: C14H19NO3
SMILES: CCCOC(=O)CN(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-82.28	kJ/mol	Joback Method
hf	-397.08	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	67.64	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.020		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	693.98	K	Joback Method
tc	899.30	K	Joback Method
tf	441.04	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.42	J/mol×K	693.98	Joback Method
cpg	567.33	J/mol×K	728.20	Joback Method
cpg	581.29	J/mol×K	762.42	Joback Method
cpg	594.34	J/mol×K	796.64	Joback Method
cpg	606.50	J/mol×K	830.86	Joback Method
cpg	617.81	J/mol×K	865.08	Joback Method
cpg	628.29	J/mol×K	899.30	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=U321213&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume