

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

Inchi:	InChI=1S/C14H19NO3/c1-4-9-18-13(16)10-15(3)14(17)12-8-6-5-7-11(12)2/h5-8H,4,9-10
InchiKey:	ULSWOTYDOHQDFK-UHFFFAOYSA-N
Formula:	C14H19NO3
SMILES:	CCCOC(=O)CN(C)C(=O)c1ccccc1C
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	1925.00		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/molxK	693.98	Joback Method
cpg	567.33	J/molxK	728.20	Joback Method
cpg	581.29	J/molxK	762.42	Joback Method
cpg	594.34	J/molxK	796.64	Joback Method
cpg	606.50	J/molxK	830.86	Joback Method
cpg	617.81	J/molxK	865.08	Joback Method
cpg	628.29	J/molxK	899.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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