

Sarcosine, N-(3-methylbenzoyl)-, octyl ester

Inchi:	InChI=1S/C19H29NO3/c1-4-5-6-7-8-9-13-23-18(21)15-20(3)19(22)17-12-10-11-16(2)14-
InchiKey:	LGGFBNPFBRLSEK-UHFFFAOYSA-N
Formula:	C19H29NO3
SMILES:	CCCCCCCCOC(=O)CN(C)C(=O)c1cccc(C)c1
Mol. weight [g/mol]:	319.44

Physical Properties

Property code	Value	Unit	Source
gf	-40.18	kJ/mol	Joback Method
hf	-500.28	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	78.77	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.971		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2479.00		NIST Webbook
tb	808.38	K	Joback Method
tc	1006.82	K	Joback Method
tf	497.39	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.73	J/molxK	808.38	Joback Method
cpg	848.10	J/molxK	841.45	Joback Method
cpg	863.41	J/molxK	874.53	Joback Method
cpg	877.70	J/molxK	907.60	Joback Method
cpg	891.01	J/molxK	940.67	Joback Method
cpg	903.38	J/molxK	973.74	Joback Method
cpg	914.85	J/molxK	1006.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321158&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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