Sarcosine, N-(4-ethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C19H29NO3/c1-4-6-7-8-9-14-23-18(21)15-20(3)19(22)17-12-10-16(5-2)11-13-
InchiKey: WEYAQRMBUKYARA-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1ccc(CC)cc1
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	-4.63		Crippen Method
logp	3.835		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2494.00		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/mol×K	808.38	Joback Method
cpg	848.10	J/mol×K	841.45	Joback Method
cpg	863.41	J/mol×K	874.53	Joback Method
cpg	877.70	J/mol×K	907.60	Joback Method
cpg	891.01	J/mol×K	940.67	Joback Method
cpg	903.38	J/mol×K	973.74	Joback Method
cpg	914.85	J/mol×K	1006.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U321234&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
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