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

Inchi: InChI=1S/C16H23NO3/c1-4-6-11-20-15(18)12-17(3)16(19)14-9-7-13(5-2)8-10-14/h7-10H
InchiKey: ZKECYENFRAJKMU-UHFFFAOYSA-N
Formula: C16H23NO3
SMILES: CCCCOC(=O)CN(C)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-65.44	kJ/mol	Joback Method
hf	-438.36	kJ/mol	Joback Method
hfus	38.25	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.664		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2198.00		NIST Webbook
tb	739.74	K	Joback Method
tc	940.76	K	Joback Method
tf	463.58	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.97	J/mol×K	739.74	Joback Method
cpg	676.57	J/mol×K	773.24	Joback Method
cpg	691.17	J/mol×K	806.75	Joback Method
cpg	704.83	J/mol×K	840.25	Joback Method
cpg	717.55	J/mol×K	873.75	Joback Method
cpg	729.39	J/mol×K	907.26	Joback Method
cpg	740.37	J/mol×K	940.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321230&Units=SI
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

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