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

Inchi: InChI=1S/C16H23NO3/c1-5-13-6-8-14(9-7-13)16(19)17(4)10-15(18)20-11-12(2)3/h6-9,12
InchiKey: KAPAOMLJNDMSLP-UHFFFAOYSA-N
Formula: C16H23NO3
SMILES: CCc1ccc(C(=O)N(C)CC(=O)OCC(C)C)cc1
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-67.88	kJ/mol	Joback Method
hf	-443.64	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	71.71	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.520		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	739.30	K	Joback Method
tc	943.32	K	Joback Method
tf	448.58	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.50	J/mol×K	739.30	Joback Method
cpg	677.35	J/mol×K	773.30	Joback Method
cpg	692.16	J/mol×K	807.31	Joback Method
cpg	705.98	J/mol×K	841.31	Joback Method
cpg	718.84	J/mol×K	875.32	Joback Method
cpg	730.77	J/mol×K	909.32	Joback Method
cpg	741.81	J/mol×K	943.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321229&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