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

Inchi: InChI=1S/C17H25NO3/c1-4-6-7-12-21-16(19)13-18(3)17(20)15-10-8-14(5-2)9-11-15/h8-1
InchiKey: KSRNUFIFLQETJE-UHFFFAOYSA-N
Formula: C17H25NO3
SMILES: CCCCCOC(=O)CN(C)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-57.02	kJ/mol	Joback Method
hf	-459.00	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.054		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2291.00		NIST Webbook
tb	762.62	K	Joback Method
tc	962.22	K	Joback Method
tf	474.85	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.91	J/mol×K	762.62	Joback Method
cpg	732.79	J/mol×K	795.89	Joback Method
cpg	747.65	J/mol×K	829.15	Joback Method
cpg	761.54	J/mol×K	862.42	Joback Method
cpg	774.49	J/mol×K	895.69	Joback Method
cpg	786.53	J/mol×K	928.95	Joback Method
cpg	797.70	J/mol×K	962.22	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=U321231&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