Sarcosine, N-(4-butylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H31NO3/c1-4-6-8-9-15-24-19(22)16-21(3)20(23)18-13-11-17(12-14-18)10-
InchiKey: ILEPPZWQWHOOFZ-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-31.76	kJ/mol	Joback Method
hf	-520.92	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	81.00	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.225		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	831.26	K	Joback Method
tc	1030.06	K	Joback Method
tf	508.66	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.48	J/mol×K	831.26	Joback Method
cpg	907.08	J/mol×K	864.39	Joback Method
cpg	922.59	J/mol×K	897.53	Joback Method
cpg	937.06	J/mol×K	930.66	Joback Method
cpg	950.53	J/mol×K	963.79	Joback Method
cpg	963.03	J/mol×K	996.92	Joback Method
cpg	974.62	J/mol×K	1030.06	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=U321135&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