Sarcosine, N-(4-methoxybenzoyl)-, isohexyl ester

Inchi: InChI=1S/C17H25NO4/c1-13(2)6-5-11-22-16(19)12-18(3)17(20)14-7-9-15(21-4)10-8-14/h
InchiKey: WULDZRANXCRCJV-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: COc1ccc(C(=O)N(C)CC(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-164.46	kJ/mol	Joback Method
hf	-596.50	kJ/mol	Joback Method
hfus	38.51	kJ/mol	Joback Method
hvap	76.34	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.747		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	784.60	K	Joback Method
tc	986.38	K	Joback Method
tf	482.08	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.04	J/mol×K	784.60	Joback Method
cpg	761.71	J/mol×K	818.23	Joback Method
cpg	776.30	J/mol×K	851.86	Joback Method
cpg	789.85	J/mol×K	885.49	Joback Method
cpg	802.37	J/mol×K	919.12	Joback Method
cpg	813.88	J/mol×K	952.75	Joback Method
cpg	824.42	J/mol×K	986.38	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=U321423&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