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

Inchi: InChI=1S/C17H25NO3/c1-13(2)6-5-11-21-16(19)12-18(4)17(20)15-9-7-14(3)8-10-15/h7-1

InchiKey: JSONAPCYIXTJPS-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: Cc1ccc(C(=O)N(C)CC(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-59.46	kJ/mol	Joback Method
hf	-464.28	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.046		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2266.00		NIST Webbook
tb	762.18	K	Joback Method
tc	964.50	K	Joback Method
tf	459.85	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.44	J/mol×K	762.18	Joback Method
cpg	733.54	J/mol×K	795.90	Joback Method
cpg	748.59	J/mol×K	829.62	Joback Method
cpg	762.63	J/mol×K	863.34	Joback Method
cpg	775.70	J/mol×K	897.06	Joback Method
cpg	787.82	J/mol×K	930.78	Joback Method
cpg	799.04	J/mol×K	964.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321217&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

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