N-benzylpalmitamide

Inchi: InChI=1S/C23H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-23(25)24-21-22-18-15-14-1
InchiKey: MLGPKWUKOQAAGI-UHFFFAOYSA-N
Formula: C23H39NO
SMILES: CCCCCCCCCCCCCCCC(O)=NCc1ccccc1
Mol. weight [g/mol]: 345.56
CAS: 74058-71-2

Physical Properties

Property code	Value	Unit	Source
hf	-361.32	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.624		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	2880.20		NIST Webbook
rinpol	2880.20		NIST Webbook
tb	921.06	K	Joback Method
tc	1128.10	K	Joback Method
tf	368.25 ± 0.50	K	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74058712&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

hf:	Enthalpy of formation 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