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]: 345.57

Physical Properties

Property code	Value	Unit	Source
af	1.0145		Cheméo Relay (1.0)
gf	215.66	kJ/mol	Joback Method
hf	-432.42	kJ/mol	Cheméo Relay (1.0)
hfus	56.06	kJ/mol	Joback Method
hvap	122.09	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-6.54		Cheméo Relay (1.0)
logp	6.784		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2880.20		NIST Webbook
rinpol	2880.20		NIST Webbook
tb	652.13	K	Cheméo Relay (1.0)
tc	878.65	K	Cheméo Relay (1.0)
tf	368.25 ± 0.50	K	NIST Webbook
vc	1.219	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.21	J/mol×K	856.36	Joback Method
cpg	1057.95	J/mol×K	889.20	Joback Method
cpg	1075.57	J/mol×K	922.04	Joback Method
cpg	1092.14	J/mol×K	954.88	Joback Method
cpg	1107.72	J/mol×K	987.72	Joback Method
cpg	1122.37	J/mol×K	1020.56	Joback Method

cpg	1136.15	J/mol×K	1053.40	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74058712&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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