

N-Octadecyl m-nitrobenzamide

Inchi:	InChI=1S/C25H42N2O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26-25(28)23-19
InchiKey:	MBGMGVISROGRGY-UHFFFAOYSA-N
Formula:	C25H42N2O3
SMILES:	CCCCCCCCCCCCCCCCNC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	418.61
CAS:	109799-65-7

Physical Properties

Property code	Value	Unit	Source
gf	258.42	kJ/mol	Joback Method
hf	-404.14	kJ/mol	Joback Method
hfus	72.22	kJ/mol	Joback Method
hvap	103.95	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	7.586		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
tb	1058.94	K	Joback Method
tc	1297.47	K	Joback Method
tf	656.65	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.24	J/molxK	1058.94	Joback Method
cpg	1304.13	J/molxK	1098.70	Joback Method
cpg	1319.77	J/molxK	1138.45	Joback Method
cpg	1334.28	J/molxK	1178.21	Joback Method
cpg	1347.79	J/molxK	1217.96	Joback Method
cpg	1360.40	J/molxK	1257.72	Joback Method
cpg	1372.23	J/molxK	1297.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C109799657&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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