

Propanamide, N,N-dioctyl-3-phenyl-

Inchi:	InChI=1S/C25H43NO/c1-3-5-7-9-11-16-22-26(23-17-12-10-8-6-4-2)25(27)21-20-24-18-1
InchiKey:	LSQXOICXJXOYNP-UHFFFAOYSA-N
Formula:	C25H43NO
SMILES:	CCCCCCCCN(CCCCCCCC)C(=O)CCc1ccccc1
Mol. weight [g/mol]:	373.62

Physical Properties

Property code	Value	Unit	Source
gf	253.89	kJ/mol	Joback Method
hf	-367.85	kJ/mol	Joback Method
hfus	59.17	kJ/mol	Joback Method
hvap	82.31	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.169		Crippen Method
mvol	350.900	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	864.39	K	Joback Method
tc	1060.51	K	Joback Method
tf	480.33	K	Joback Method
vc	1.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.72	J/molxK	864.39	Joback Method
cpg	1161.77	J/molxK	897.08	Joback Method
cpg	1180.66	J/molxK	929.76	Joback Method
cpg	1198.45	J/molxK	962.45	Joback Method
cpg	1215.22	J/molxK	995.14	Joback Method
cpg	1231.03	J/molxK	1027.83	Joback Method
cpg	1245.96	J/molxK	1060.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/44-510-6/Propanamide-N-N-dioctyl-3-phenyl.pdf>

Generated by Cheméo on 2024-04-25 16:06:38.486714541 +0000 UTC m=+16350447.407291851.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.