

Benzamide, 4-methyl-N-octadecyl-

Inchi: InChI=1S/C26H45NO/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-27-26(28)25-21-
InchiKey: BMEUJBGSXIGPTC-UHFFFAOYSA-N
Formula: C26H45NO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 387.64

Physical Properties

Property code	Value	Unit	Source
gf	231.29	kJ/mol	Joback Method
hf	-414.02	kJ/mol	Joback Method
hfus	63.45	kJ/mol	Joback Method
hvap	89.59	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	7.986		Crippen Method
mcvol	364.990	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook
tb	929.98	K	Joback Method
tc	1138.58	K	Joback Method
tf	524.31	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.49	J/mol×K	929.98	Joback Method
cpg	1246.26	J/mol×K	964.75	Joback Method
cpg	1264.79	J/mol×K	999.51	Joback Method
cpg	1282.14	J/mol×K	1034.28	Joback Method
cpg	1298.39	J/mol×K	1069.05	Joback Method
cpg	1313.63	J/mol×K	1103.81	Joback Method
cpg	1327.93	J/mol×K	1138.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407480&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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