

# Benzamide, N-heptyl-N-octyl-4-trifluoromethyl-

<b>Inchi:</b>	InChI=1S/C23H36F3NO/c1-3-5-7-9-11-13-19-27(18-12-10-8-6-4-2)22(28)20-14-16-21(17)
<b>InchiKey:</b>	AWHNZGKBQITTBW-UHFFFAOYSA-N
<b>Formula:</b>	C23H36F3NO
<b>SMILES:</b>	CCCCCCCCN(CCCCCC)C(=O)c1ccc(C(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	399.53

## Physical Properties

Property code	Value	Unit	Source
gf	-354.17	kJ/mol	Joback Method
hf	-935.12	kJ/mol	Joback Method
hfus	55.42	kJ/mol	Joback Method
hvap	74.77	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.479		Crippen Method
mvol	328.030	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	2386.00		NIST Webbook
tb	818.19	K	Joback Method
tc	1005.06	K	Joback Method
tf	474.50	K	Joback Method
vc	1.282	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.60	J/molxK	818.19	Joback Method
cpg	1058.92	J/molxK	849.33	Joback Method
cpg	1076.20	J/molxK	880.48	Joback Method
cpg	1092.51	J/molxK	911.62	Joback Method
cpg	1107.91	J/molxK	942.77	Joback Method
cpg	1122.48	J/molxK	973.91	Joback Method
cpg	1136.28	J/molxK	1005.06	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308253&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308253&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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