

# Benzamide, 3-trifluoromethyl-2-fluoro-N-hexadecyl-

Inchi:	InChI=1S/C24H37F4NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-29-23(30)20-17-16-18
InchiKey:	BTOBHZQEYMMOOR-UHFFFAOYSA-N
Formula:	C24H37F4NO
SMILES:	CCCCCCCCCCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	431.55

## Physical Properties

Property code	Value	Unit	Source
gf	-571.58	kJ/mol	Joback Method
hf	-1177.40	kJ/mol	Joback Method
hfus	62.78	kJ/mol	Joback Method
hvap	81.24	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.056		Crippen Method
mvol	343.890	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	2736.00		NIST Webbook
rinpol	2736.00		NIST Webbook
tb	883.05	K	Joback Method
tc	1081.10	K	Joback Method
tf	519.07	K	Joback Method
vc	1.373	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.53	J/molxK	883.05	Joback Method
cpg	1147.52	J/molxK	916.06	Joback Method
cpg	1164.42	J/molxK	949.07	Joback Method
cpg	1180.33	J/molxK	982.08	Joback Method
cpg	1195.30	J/molxK	1015.09	Joback Method
cpg	1209.41	J/molxK	1048.09	Joback Method
cpg	1222.74	J/molxK	1081.10	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<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=U407714&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407714&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>

# 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>hvap:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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