

# trans-Cinnamamide, n-heptyl-n-octyl-3-trifluoromethyl-

<b>Inchi:</b>	InChI=1S/C25H38F3NO/c1-3-5-7-9-11-13-20-29(19-12-10-8-6-4-2)24(30)18-17-22-15-14
<b>InchiKey:</b>	BQDWRC AUWXEUTQ-ISLYRVAYSA-N
<b>Formula:</b>	C25H38F3NO
<b>SMILES:</b>	CCCCCCCCN(CCCCCC)C(=O)C=Cc1ccc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	425.57

## Physical Properties

Property code	Value	Unit	Source
gf	-257.11	kJ/mol	Joback Method
hf	-859.18	kJ/mol	Joback Method
hfus	60.81	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.878		Crippen Method
mvol	351.910	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	2725.00		NIST Webbook
rinpol	2725.00		NIST Webbook
tb	868.11	K	Joback Method
tc	1063.72	K	Joback Method
tf	491.96	K	Joback Method
vc	1.375	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.20	J/mol×K	868.11	Joback Method
cpg	1155.83	J/mol×K	900.71	Joback Method
cpg	1173.44	J/mol×K	933.31	Joback Method
cpg	1190.13	J/mol×K	965.92	Joback Method
cpg	1205.98	J/mol×K	998.52	Joback Method
cpg	1221.10	J/mol×K	1031.12	Joback Method
cpg	1235.57	J/mol×K	1063.72	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308075&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308075&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</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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