

# trans-Cinnamamide, N,N-bis(2-ethylhexyl)-3-trifluoromethyl-

Inchi:	InChI=1S/C26H40F3NO/c1-5-9-12-21(7-3)19-30(20-22(8-4)13-10-6-2)25(31)17-16-23-14
InchiKey:	PQRZKBDCCGKQFU-WUKNDPDISA-N
Formula:	C26H40F3NO
SMILES:	CCCCC(CC)CN(CC(CC)CCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	439.60

## Physical Properties

Property code	Value	Unit	Source
gf	-253.57	kJ/mol	Joback Method
hf	-890.38	kJ/mol	Joback Method
hfus	56.35	kJ/mol	Joback Method
hvap	80.63	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.980		Crippen Method
mcvol	366.000	ml/mol	McGowan Method
pc	872.74	kPa	Joback Method
rinsol	2573.00		NIST Webbook
tb	890.11	K	Joback Method
tc	1090.40	K	Joback Method
tf	473.23	K	Joback Method
vc	1.419	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.23	J/molxK	890.11	Joback Method
cpg	1219.36	J/molxK	923.49	Joback Method
cpg	1237.43	J/molxK	956.87	Joback Method
cpg	1254.53	J/molxK	990.26	Joback Method
cpg	1270.76	J/molxK	1023.64	Joback Method
cpg	1286.24	J/molxK	1057.02	Joback Method
cpg	1301.07	J/molxK	1090.40	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308073&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>

# 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>hvac:</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>mccol:</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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