trans-Cinnamamide, N,N-dihexyl-3-trifluoromethyl-

Inchi: InChI=1S/C22H32F3NO/c1-3-5-7-9-16-26(17-10-8-6-4-2)21(27)15-14-19-12-11-13-20(18

InchiKey: WPLWCFFJRJYKCV-CCEZHUSRSA-N

Formula: C22H32F3NO

SMILES: CCCCCCN(CCCCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 383.49

Physical Properties

Property code	Value	Unit	Source
gf	-282.37	kJ/mol	Joback Method
hf	-797.26	kJ/mol	Joback Method
hfus	53.04	kJ/mol	Joback Method
hvap	72.50	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.708		Crippen Method
mcvol	309.640	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	799.47	K	Joback Method
tc	987.14	K	Joback Method
tf	458.15	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.17	J/mol×K	799.47	Joback Method
cpg	972.60	J/mol×K	830.75	Joback Method
cpg	989.05	J/mol×K	862.03	Joback Method
cpg	1004.61	J/mol×K	893.31	Joback Method
cpg	1019.33	J/mol×K	924.58	Joback Method
cpg	1033.31	J/mol×K	955.86	Joback Method
cpg	1046.62	J/mol×K	987.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308071&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume