trans-Cinnamamide, N,N-dioctyl-3-trifluoromethyl-

Inchi: InChI=1S/C26H40F3NO/c1-3-5-7-9-11-13-20-30(21-14-12-10-8-6-4-2)25(31)19-18-23-16

InchiKey: KNZBFZBYARYENM-VHEBQXMUSA-N

Formula: C26H40F3NO

SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 439.60

Physical Properties

Property code	Value	Unit	Source
gf	-248.69	kJ/mol	Joback Method
hf	-879.82	kJ/mol	Joback Method
hfus	63.40	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.268		Crippen Method
mcvol	366.000	ml/mol	McGowan Method
pc	864.54	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	890.99	K	Joback Method
tc	1090.90	K	Joback Method
tf	503.23	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.35	J/mol×K	890.99	Joback Method
cpg	1218.49	J/mol×K	924.31	Joback Method
cpg	1236.59	J/mol×K	957.63	Joback Method
cpg	1253.76	J/mol×K	990.94	Joback Method
cpg	1270.09	J/mol×K	1024.26	Joback Method
cpg	1285.68	J/mol×K	1057.58	Joback Method
cpg	1300.65	J/mol×K	1090.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308076&Units=SI
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

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