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=C/c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 439.61

Physical Properties

Property code	Value	Unit	Source
hfus	56.35	kJ/mol	Joback Method
ie	8.20	eV	Cheméo Relay (1.0)
logp	7.980		Crippen Method
mcvol	366.000	ml/mol	McGowan Method
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook

Temperature Dependent Properties

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

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308073&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices