trans-Cinnamamide, N,N-dinonyl-3-trifluoromethyl-

Inchi: InChI=1S/C28H44F3NO/c1-3-5-7-9-11-13-15-22-32(23-16-14-12-10-8-6-4-2)27(33)21-20

InchiKey: ZYRMMQSHGBCTJJ-QZQOTICOSA-N

Formula: C28H44F3NO

SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 467.65

Physical Properties

Property code	Value	Unit	Source
gf	-231.85	kJ/mol	Joback Method
hf	-921.10	kJ/mol	Joback Method
hfus	68.58	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	9.048		Crippen Method
mcvol	394.180	ml/mol	McGowan Method
pc	774.61	kPa	Joback Method
rinpol	3071.00		NIST Webbook
tb	936.75	K	Joback Method
tc	1148.13	K	Joback Method
tf	525.77	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1325.62	J/mol×K	936.75	Joback Method
cpg	1346.02	J/mol×K	971.98	Joback Method
cpg	1365.32	J/mol×K	1007.21	Joback Method
cpg	1383.65	J/mol×K	1042.44	Joback Method
cpg	1401.14	J/mol×K	1077.67	Joback Method
cpg	1417.92	J/mol×K	1112.90	Joback Method
cpg	1434.11	J/mol×K	1148.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308077&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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