trans-Cinnamamide, n-decyl-N-methyl-3-trifluoromethyl-

Inchi: InChI=1S/C21H30F3NO/c1-3-4-5-6-7-8-9-10-16-25(2)20(26)15-14-18-12-11-13-19(17-18

InchiKey: ZMGRFNXTKZZOBA-CCEZHUSRSA-N

Formula: C21H30F3NO

SMILES: CCCCCCCCCCN(C)C(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 369.46

Physical Properties

Property code	Value	Unit	Source
gf	-290.79	kJ/mol	Joback Method
hf	-776.62	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	70.28	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.318		Crippen Method
mcvol	295.550	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	2482.00		NIST Webbook
tb	776.59	K	Joback Method
tc	963.05	K	Joback Method
tf	446.88	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.12	J/mol×K	776.59	Joback Method
cpg	913.23	J/mol×K	807.67	Joback Method
cpg	929.37	J/mol×K	838.74	Joback Method
cpg	944.61	J/mol×K	869.82	Joback Method
cpg	959.03	J/mol×K	900.90	Joback Method
cpg	972.69	J/mol×K	931.98	Joback Method
cpg	985.67	J/mol×K	963.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308072&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

Latest version available from:
https://www.chemeo.com/cid/44-441-3/trans-Cinnamamide-n-decyl-N-methyl-3-trifluoromethyl.pdf
Generated by Cheméo on 2024-10-12 04:31:50.61704336 +0000 UTC m=+3288373.254012609.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.