trans-Cinnamamide, N-(3-chlorophenyl)-3-trifluoromethyl-

Inchi: InChI=1S/C16H11ClF3NO/c17-13-5-2-6-14(10-13)21-15(22)8-7-11-3-1-4-12(9-11)16(18,

InchiKey: SMMFWYAGPPOQMC-BQYQJAHWSA-N

Formula: C16H11ClF3NO

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Nc1cccc(Cl)c1

Mol. weight [g/mol]: 325.71

Physical Properties

Property code	Value	Unit	Source
gf	-263.43	kJ/mol	Joback Method
hf	-478.16	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.011		Crippen Method
mcvol	213.580	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	2471.00		NIST Webbook
tb	769.01	K	Joback Method
tc	998.46	K	Joback Method
tf	479.58	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.81	J/mol×K	769.01	Joback Method
cpg	580.72	J/mol×K	807.25	Joback Method
cpg	591.64	J/mol×K	845.49	Joback Method
cpg	601.68	J/mol×K	883.74	Joback Method
cpg	610.95	J/mol×K	921.98	Joback Method
cpg	619.56	J/mol×K	960.22	Joback Method
cpg	627.62	J/mol×K	998.46	Joback Method

Sources

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=U307370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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