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

Inchi: InChI=1S/C17H14F3NO/c1-12-4-2-7-15(10-12)21-16(22)9-8-13-5-3-6-14(11-13)17(18,19

InchiKey: XYPIIKLMVAJECA-CMDGGOBGSA-N

Formula: C17H14F3NO

SMILES: Cc1cccc(NC(=O)C=Cc2cccc(C(F)(F)F)c2)c1

Mol. weight [g/mol]: 305.29

Physical Properties

Property code	Value	Unit	Source
gf	-243.08	kJ/mol	Joback Method
hf	-483.06	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.666		Crippen Method
mcvol	215.430	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	754.46	K	Joback Method
tc	977.62	K	Joback Method
tf	460.93	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.65	J/mol×K	754.46	Joback Method
cpg	612.16	J/mol×K	791.65	Joback Method
cpg	624.61	J/mol×K	828.85	Joback Method
cpg	636.12	J/mol×K	866.04	Joback Method
cpg	646.77	J/mol×K	903.23	Joback Method
cpg	656.68	J/mol×K	940.42	Joback Method
cpg	665.94	J/mol×K	977.62	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=U307369&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