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

Inchi: InChI=1S/C19H18F3NO/c1-3-23(17-9-4-6-14(2)12-17)18(24)11-10-15-7-5-8-16(13-15)19

InchiKey: YASSUSJXRYJNOU-ZHACJKMWSA-N

Formula: C19H18F3NO

SMILES: CCN(C(=O)C=Cc1cccc(C(F)(F)F)c1)c1cccc(C)c1

Mol. weight [g/mol]: 333.35

Physical Properties

Property code	Value	Unit	Source
gf	-204.85	kJ/mol	Joback Method
hf	-510.28	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	68.76	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.080		Crippen Method
mcvol	243.610	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	762.49	K	Joback Method
tc	977.58	K	Joback Method
tf	463.28	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.63	J/mol×K	762.49	Joback Method
cpg	708.62	J/mol×K	798.34	Joback Method
cpg	722.51	J/mol×K	834.19	Joback Method
cpg	735.42	J/mol×K	870.03	Joback Method
cpg	747.44	J/mol×K	905.88	Joback Method
cpg	758.68	J/mol×K	941.73	Joback Method
cpg	769.25	J/mol×K	977.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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