trans-Cinnamamide, N-(4-methoxyphenyl)-3-trifluoromethyl-

Inchi: InChI=1S/C17H14F3NO2/c1-23-15-8-6-14(7-9-15)21-16(22)10-5-12-3-2-4-13(11-12)17(1

InchiKey: CBNQBQRHCQWJHR-BJMVGYQFSA-N

Formula: C17H14F3NO2

SMILES: COc1ccc(NC(=O)C=Cc2cccc(C(F)(F)F)c2)cc1

Mol. weight [g/mol]: 321.29

Physical Properties

Property code	Value	Unit	Source
gf	-348.08	kJ/mol	Joback Method
hf	-615.28	kJ/mol	Joback Method
hfus	37.00	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.366		Crippen Method
mcvol	221.300	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	776.88	K	Joback Method
tc	997.81	K	Joback Method
tf	483.16	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.62	J/mol×K	776.88	Joback Method
cpg	637.71	J/mol×K	813.70	Joback Method
cpg	649.76	J/mol×K	850.52	Joback Method
cpg	660.85	J/mol×K	887.34	Joback Method
cpg	671.08	J/mol×K	924.17	Joback Method
cpg	680.52	J/mol×K	960.99	Joback Method
cpg	689.25	J/mol×K	997.81	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=U307371&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