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

Inchi: InChI=1S/C16H11F4NO/c17-13-5-7-14(8-6-13)21-15(22)9-4-11-2-1-3-12(10-11)16(18,19

InchiKey: UTZMZDANOHXJIL-RUDMXATFSA-N

Formula: C16H11F4NO

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Nc1ccc(F)cc1

Mol. weight [g/mol]: 309.26

Physical Properties

Property code	Value	Unit	Source
gf	-446.31	kJ/mol	Joback Method
hf	-658.53	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	65.66	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.496		Crippen Method
mcvol	203.110	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	2244.00		NIST Webbook
tb	730.85	K	Joback Method
tc	948.60	K	Joback Method
tf	450.25	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.50	J/mol×K	730.85	Joback Method
cpg	566.06	J/mol×K	767.14	Joback Method
cpg	577.61	J/mol×K	803.43	Joback Method
cpg	588.26	J/mol×K	839.72	Joback Method
cpg	598.08	J/mol×K	876.02	Joback Method
cpg	607.18	J/mol×K	912.31	Joback Method
cpg	615.64	J/mol×K	948.60	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=U307368&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

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