trans-Cinnamamide, N-tetrahydrofurfuryl-3-trifluoromethyl-

Inchi: InChI=1S/C15H16F3NO2/c16-15(17,18)12-4-1-3-11(9-12)6-7-14(20)19-10-13-5-2-8-21-1

InchiKey: HPOVVGRSTIYLPV-VOTSOKGWSA-N

Formula: C15H16F3NO2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)NCC1CCCO1

Mol. weight [g/mol]: 299.29

Physical Properties

Property code	Value	Unit	Source
gf	-412.27	kJ/mol	Joback Method
hf	-738.36	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	66.08	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.014		Crippen Method
mcvol	206.020	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	719.27	K	Joback Method
tc	934.41	K	Joback Method
tf	436.92	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.92	J/mol×K	719.27	Joback Method
cpg	615.01	J/mol×K	755.13	Joback Method
cpg	628.96	J/mol×K	790.98	Joback Method
cpg	641.86	J/mol×K	826.84	Joback Method
cpg	653.82	J/mol×K	862.69	Joback Method
cpg	664.91	J/mol×K	898.55	Joback Method
cpg	675.24	J/mol×K	934.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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