cis-«alpha»-Phenylcinnamamide

Inchi: InChI=1S/C15H13NO/c16-15(17)14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-11H,(H2,16
InchiKey: VTOAFAPBGXLGME-KAMYIIQDSA-N
Formula: C15H13NO
SMILES: N=C(O)C(=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 223.27
CAS: 20432-29-5

Physical Properties

Property code	Value	Unit	Source
gf	438.69	kJ/mol	Joback Method
hf	273.66	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	3.762		Crippen Method
mcvol	181.940	ml/mol	McGowan Method
tb	776.52	K	Joback Method
tf	422.21	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.68	J/mol×K	776.52	Joback Method
cpg	24.26	J/mol×K	100.12	Joback Method
cpg	24.26	J/mol×K	100.12	Joback Method
cpg	24.26	J/mol×K	100.12	Joback Method
cpg	24.26	J/mol×K	100.12	Joback Method
cpg	24.26	J/mol×K	100.12	Joback Method
cpg	24.26	J/mol×K	100.12	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=C20432295&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point