

trans-Amyl cinnamate

Inchi:	InChI=1S/C14H18O2/c1-2-3-7-12-16-14(15)11-10-13-8-5-4-6-9-13/h4-6,8-11H,2-3,7,12H
InchiKey:	QDRJCWZGTMRXCL-ZHACJKMWSA-N
Formula:	C14H18O2
SMILES:	CCCCCOC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	25.71	kJ/mol	Joback Method
hf	-223.34	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	58.15	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.433		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
ripol	2356.00		NIST Webbook
tb	626.85	K	Joback Method
tc	834.90	K	Joback Method
tf	341.04	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.32	J/mol×K	626.85	Joback Method
cpg	489.16	J/mol×K	661.52	Joback Method
cpg	504.05	J/mol×K	696.20	Joback Method
cpg	518.03	J/mol×K	730.87	Joback Method
cpg	531.13	J/mol×K	765.55	Joback Method
cpg	543.41	J/mol×K	800.22	Joback Method
cpg	554.89	J/mol×K	834.90	Joback Method
dvisc	0.0019011	Paxs	341.04	Joback Method
dvisc	0.0009243	Paxs	388.68	Joback Method

dvisc	0.0005261	Paxs	436.31	Joback Method
dvisc	0.0003345	Paxs	483.95	Joback Method
dvisc	0.0002307	Paxs	531.58	Joback Method
dvisc	0.0001691	Paxs	579.22	Joback Method
dvisc	0.0001300	Paxs	626.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/71-895-0/trans-Amyl-cinnamate.pdf>

Generated by Cheméo on 2024-04-28 01:24:42.262259256 +0000 UTC m=+16556731.182836568.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.