

trans-Ethyl p-methoxycinnamate

Inchi:	InChI=1S/C12H14O3/c1-3-15-12(13)9-6-10-4-7-11(14-2)8-5-10/h4-9H,3H2,1-2H3/b9-6+
InchiKey:	DHNGCHLFKUPGPX-RMKNXTFCSA-N
Formula:	C12H14O3
SMILES:	CCOC(=O)C=Cc1ccc(OC)cc1
Mol. weight [g/mol]:	206.24

Physical Properties

Property code	Value	Unit	Source
gf	-105.76	kJ/mol	Joback Method
hf	-325.75	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.272		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1765.00		NIST Webbook
tb	608.49	K	Joback Method
tc	821.95	K	Joback Method
tf	353.25	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.77	J/molxK	608.49	Joback Method
cpg	461.38	J/molxK	786.38	Joback Method
cpg	450.41	J/molxK	750.80	Joback Method
cpg	438.68	J/molxK	715.22	Joback Method
cpg	426.17	J/molxK	679.64	Joback Method
cpg	412.88	J/molxK	644.07	Joback Method
cpg	471.62	J/molxK	821.95	Joback Method
dvisc	0.0001240	Paxs	608.49	Joback Method
dvisc	0.0001566	Paxs	565.95	Joback Method

dvisc	0.0002054	Paxs	523.41	Joback Method
dvisc	0.0002826	Paxs	480.87	Joback Method
dvisc	0.0004138	Paxs	438.33	Joback Method
dvisc	0.0006576	Paxs	395.79	Joback Method
dvisc	0.0011684	Paxs	353.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R576553&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

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
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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