trans-Cinnamyl tiglate

Other names: (2E)-3-Phenyl-2-propenyl (2E)-2-methyl-2-butenoate
(E)-Cinnamyl tiglate
2-Butenoic acid, 2-methyl-, 3-phenyl-2-propenyl ester, (E,E)-
Inchi: InChI=1S/C14H16O2/c1-3-12(2)14(15)16-11-7-10-13-8-5-4-6-9-13/h3-10H,11H2,1-2H3/b
InchiKey: KRNURAJANZKGQN-IBIBRXRCSA-N
Formula: C14H16O2
SMILES: CC=C(C)C(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 216.28
CAS: 72934-01-1

Physical Properties

Property code	Value	Unit	Source
gf	97.38	kJ/mol	Joback Method
hf	-115.91	kJ/mol	Joback Method
hfus	27.94	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.209		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
ripol	2556.00		NIST Webbook
ripol	2556.00		NIST Webbook
tb	630.89	K	Joback Method
tc	851.13	K	Joback Method
tf	322.00	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.00	J/mol×K	630.89	Joback Method
cpg	467.53	J/mol×K	667.60	Joback Method
cpg	482.04	J/mol×K	704.30	Joback Method
cpg	495.58	J/mol×K	741.01	Joback Method

cpg	508.22	J/mol×K	777.72	Joback Method
cpg	520.02	J/mol×K	814.43	Joback Method
cpg	531.05	J/mol×K	851.13	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=C72934011&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
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