Butanoic acid, 3-methyl-, 3-phenyl-2-propenyl ester

Other names: Isovaleric acid, cinnamyl ester
Cinnamyl isovalerate
3-Phenylallyl isovalerate

Inchi: InChI=1S/C14H18O2/c1-12(2)11-14(15)16-10-6-9-13-7-4-3-5-8-13/h3-9,12H,10-11H2,1-2

InchiKey: FOCMOGKCPPTERB-RMKNXTFCSA-N

Formula: C14H18O2

SMILES: CC(C)CC(=O)OCC=Cc1ccccc1

Mol. weight [g/mol]: 218.29

CAS: 140-27-2

Physical Properties

Property code	Value	Unit	Source
gf	23.27	kJ/mol	Joback Method
hf	-228.62	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.289		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1655.00		NIST Webbook
ripol	2289.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2289.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2289.00		NIST Webbook
tb	626.41	K	Joback Method
tc	838.56	K	Joback Method
tf	326.04	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.76	J/mol×K	626.41	Joback Method
cpg	489.96	J/mol×K	661.77	Joback Method
cpg	505.16	J/mol×K	697.13	Joback Method
cpg	519.40	J/mol×K	732.49	Joback Method
cpg	532.72	J/mol×K	767.84	Joback Method
cpg	545.17	J/mol×K	803.20	Joback Method
cpg	556.80	J/mol×K	838.56	Joback Method
dvisc	0.0024476	Pa×s	326.04	Joback Method
dvisc	0.0010623	Pa×s	376.10	Joback Method
dvisc	0.0005610	Pa×s	426.16	Joback Method
dvisc	0.0003388	Pa×s	476.23	Joback Method
dvisc	0.0002252	Pa×s	526.29	Joback Method
dvisc	0.0001607	Pa×s	576.35	Joback Method
dvisc	0.0001210	Pa×s	626.41	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C140272&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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