ISOVALERIC ACID, 3-PHENYLPROPYL ESTER

Other names: Isovaleric acid, 3-phenylpropyl ester
3-Phenylpropyl 3-methylbutanoate
3-phenylpropyl isovalerate
Inchi: InChI=1S/C14H20O2/c1-12(2)11-14(15)16-10-6-9-13-7-4-3-5-8-13/h3-5,7-8,12H,6,9-11H
InchiKey: LBNFCOMOXOWXCD-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CC(C)CC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
af	0.6307		Cheméo Relay (1.0)
gf	-56.95	kJ/mol	Joback Method
hf	-413.05	kJ/mol	Cheméo Relay (1.0)
hfus	25.32	kJ/mol	Joback Method
hvap	73.13	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-3.70		Cheméo Relay (1.0)
logp	3.209		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1590.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	529.44	K	Cheméo Relay (1.0)
tc	754.97	K	Cheméo Relay (1.0)
tf	251.85	K	Cheméo Relay (1.0)
vc	0.707	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.55	J/mol×K	622.25	Joback Method
cpg	580.93	J/mol×K	826.14	Joback Method
cpg	568.74	J/mol×K	792.16	Joback Method
cpg	555.70	J/mol×K	758.18	Joback Method
cpg	541.79	J/mol×K	724.20	Joback Method
cpg	526.98	J/mol×K	690.21	Joback Method
cpg	511.24	J/mol×K	656.23	Joback Method
dvisc	0.0003900	Pa×s	476.69	Joback Method
dvisc	0.0001414	Pa×s	622.25	Joback Method
dvisc	0.0001872	Pa×s	573.73	Joback Method
dvisc	0.0002612	Pa×s	525.21	Joback Method
dvisc	0.0026271	Pa×s	331.12	Joback Method
dvisc	0.0006378	Pa×s	428.16	Joback Method
dvisc	0.0011824	Pa×s	379.64	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5452073&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie:	Ionization energy
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