

Butanoic acid, 3-methyl-, 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)OCCc1ccccc1
Mol. weight [g/mol]:	220.31
CAS:	5452-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-56.95	kJ/mol	Joback Method
hf	-345.84	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	57.80	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.208		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
ripol	2100.00		NIST Webbook
tb	622.25	K	Joback Method
tc	826.14	K	Joback Method
tf	331.12	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.55	J/mol×K	622.25	Joback Method
cpg	511.24	J/mol×K	656.23	Joback Method
cpg	526.98	J/mol×K	690.21	Joback Method

cpg	541.79	J/molxK	724.20	Joback Method
cpg	555.70	J/molxK	758.18	Joback Method
cpg	568.74	J/molxK	792.16	Joback Method
cpg	580.93	J/molxK	826.14	Joback Method
dvisc	0.0026271	Paxs	331.12	Joback Method
dvisc	0.0011824	Paxs	379.64	Joback Method
dvisc	0.0006378	Paxs	428.16	Joback Method
dvisc	0.0003900	Paxs	476.69	Joback Method
dvisc	0.0002612	Paxs	525.21	Joback Method
dvisc	0.0001872	Paxs	573.73	Joback Method
dvisc	0.0001414	Paxs	622.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5452073&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
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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