Butyric acid, 3-methyl-3-[2-isopropylphenyl]-

Inchi: InChI=1S/C14H20O2/c1-10(2)11-7-5-6-8-12(11)14(3,4)9-13(15)16/h5-8,10H,9H2,1-4H3,(
InchiKey: DXOMBIDMLJEHGO-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CC(C)c1ccccc1C(C)(C)CC(=O)O
Mol. weight [g/mol]: 220.31
CAS: 92300-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-95.56	kJ/mol	Joback Method
hf	-386.07	kJ/mol	Joback Method
hfus	20.42	kJ/mol	Joback Method
hvap	71.44	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.562		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
tb	693.76	K	Joback Method
tc	898.12	K	Joback Method
tf	384.65	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.43	J/mol×K	693.76	Joback Method
cpg	544.59	J/mol×K	727.82	Joback Method
cpg	557.84	J/mol×K	761.88	Joback Method
cpg	570.25	J/mol×K	795.94	Joback Method
cpg	581.85	J/mol×K	830.00	Joback Method
cpg	592.71	J/mol×K	864.06	Joback Method
cpg	602.89	J/mol×K	898.12	Joback Method

dvisc	0.0031609	Pa×s	384.65	Joback Method
dvisc	0.0009676	Pa×s	436.17	Joback Method
dvisc	0.0003804	Pa×s	487.69	Joback Method
dvisc	0.0001787	Pa×s	539.21	Joback Method
dvisc	0.0000958	Pa×s	590.72	Joback Method
dvisc	0.0000568	Pa×s	642.24	Joback Method
dvisc	0.0000364	Pa×s	693.76	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=C92300817&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
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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