Butanoic acid, 2-methyl-, phenylmethyl ester

Other names: Benzyl 2-methylbutyrate
Benzyl 2-methylbutanoate
Inchi: InChI=1S/C12H16O2/c1-3-10(2)12(13)14-9-11-7-5-4-6-8-11/h4-8,10H,3,9H2,1-2H3
InchiKey: PTKDIBUNVYIPOD-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CCC(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]: 192.25
CAS: 56423-40-6

Physical Properties

Property code	Value	Unit	Source
gf	-73.79	kJ/mol	Joback Method
hf	-304.56	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.776		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1880.00		NIST Webbook
tb	576.49	K	Joback Method
tc	786.80	K	Joback Method
tf	308.58	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	394.41	J/mol×K	576.49	Joback Method
cpg	463.49	J/mol×K	751.74	Joback Method
cpg	451.37	J/mol×K	716.69	Joback Method
cpg	438.42	J/mol×K	681.64	Joback Method
cpg	424.63	J/mol×K	646.59	Joback Method
cpg	409.96	J/mol×K	611.54	Joback Method
cpg	474.82	J/mol×K	786.80	Joback Method
dvisc	0.0001725	Pa×s	576.49	Joback Method
dvisc	0.0002268	Pa×s	531.84	Joback Method
dvisc	0.0003136	Pa×s	487.19	Joback Method
dvisc	0.0004628	Pa×s	442.54	Joback Method
dvisc	0.0007455	Pa×s	397.88	Joback Method
dvisc	0.0013546	Pa×s	353.23	Joback Method
dvisc	0.0029260	Pa×s	308.58	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=C56423406&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