Benzoic acid, 4-methyl, 3-methylbutyl ester

Other names: p-Toluic acid, 3-methylbutyl ester
4-Methylbenzoic acid, 3-methylbutyl ester
Inchi: InChI=1S/C13H18O2/c1-10(2)8-9-15-13(14)12-6-4-11(3)5-7-12/h4-7,10H,8-9H2,1-3H3
InchiKey: WDNOGGRIGNCXKH-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: Cc1ccc(C(=O)OCCC(C)C)cc1
Mol. weight [g/mol]: 206.28
CAS: 331810-91-4

Physical Properties

Property code	Value	Unit	Source
gf	-75.00	kJ/mol	Joback Method
hf	-336.67	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.198		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1591.00		NIST Webbook
tb	604.35	K	Joback Method
tc	812.28	K	Joback Method
tf	332.37	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.45	J/mol×K	604.35	Joback Method
cpg	514.48	J/mol×K	777.63	Joback Method
cpg	501.96	J/mol×K	742.97	Joback Method
cpg	488.62	J/mol×K	708.32	Joback Method
cpg	474.43	J/mol×K	673.66	Joback Method
cpg	459.38	J/mol×K	639.01	Joback Method

cpg	526.19	J/mol×K	812.28	Joback Method
dvisc	0.0001539	Pa×s	604.35	Joback Method
dvisc	0.0001992	Pa×s	559.02	Joback Method
dvisc	0.0002698	Pa×s	513.69	Joback Method
dvisc	0.0003877	Pa×s	468.36	Joback Method
dvisc	0.0006019	Pa×s	423.03	Joback Method
dvisc	0.0010385	Pa×s	377.70	Joback Method
dvisc	0.0020794	Pa×s	332.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C331810914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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