4-Methylbenzoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C14H20O2/c1-4-5-12(3)10-16-14(15)13-8-6-11(2)7-9-13/h6-9,12H,4-5,10H2,1-
InchiKey: AEQFYDMELOAHTJ-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCC(C)COC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	-66.58	kJ/mol	Joback Method
hf	-357.31	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.588		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1691.00		NIST Webbook
tb	627.23	K	Joback Method
tc	832.03	K	Joback Method
tf	343.64	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.28	J/mol×K	627.23	Joback Method
cpg	510.76	J/mol×K	661.36	Joback Method
cpg	526.32	J/mol×K	695.50	Joback Method
cpg	540.99	J/mol×K	729.63	Joback Method
cpg	554.78	J/mol×K	763.76	Joback Method
cpg	567.73	J/mol×K	797.90	Joback Method
cpg	579.84	J/mol×K	832.03	Joback Method
dvisc	0.0019801	Pa×s	343.64	Joback Method
dvisc	0.0009738	Pa×s	390.90	Joback Method

dvisc	0.0005582	Pa×s	438.17	Joback Method
dvisc	0.0003565	Pa×s	485.44	Joback Method
dvisc	0.0002466	Pa×s	532.70	Joback Method
dvisc	0.0001811	Pa×s	579.97	Joback Method
dvisc	0.0001394	Pa×s	627.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354152&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume