Benzoic acid, hept-2-yl ester

Other names: 2-Heptanol, benzoate
Inchi: InChI=1S/C14H20O2/c1-3-4-6-9-12(2)16-14(15)13-10-7-5-8-11-13/h5,7-8,10-12H,3-4,6,9
InchiKey: WMGISUKBJZWCDP-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCCC(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 220.31

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	-4.34		Crippen Method
logp	3.812		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1610.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2034.00		NIST Webbook
tb	622.25	K	Joback Method
tc	826.14	K	Joback Method
tf	331.12	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	494.55	J/mol×K	622.25	Joback Method
cpg	568.74	J/mol×K	792.16	Joback Method
cpg	555.70	J/mol×K	758.18	Joback Method
cpg	541.79	J/mol×K	724.20	Joback Method
cpg	526.98	J/mol×K	690.21	Joback Method
cpg	511.24	J/mol×K	656.23	Joback Method
cpg	580.93	J/mol×K	826.14	Joback Method
dvisc	0.0001414	Pa×s	622.25	Joback Method
dvisc	0.0001872	Pa×s	573.73	Joback Method
dvisc	0.0002612	Pa×s	525.21	Joback Method
dvisc	0.0003900	Pa×s	476.69	Joback Method
dvisc	0.0006378	Pa×s	428.16	Joback Method
dvisc	0.0011824	Pa×s	379.64	Joback Method
dvisc	0.0026271	Pa×s	331.12	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368694&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume