Benzoic acid, hept-3-yl ester

Inchi: InChI=1S/C14H20O2/c1-3-5-11-13(4-2)16-14(15)12-9-7-6-8-10-12/h6-10,13H,3-5,11H2,1
InchiKey: QBMDOZADPSFEBH-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCC(CC)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	1587.00		NIST Webbook
rinpol	1587.00		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=U368767&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