Propyl 3-(2-hydroxyphenyl)propanoate

Inchi: InChI=1S/C12H16O3/c1-2-9-15-12(14)8-7-10-5-3-4-6-11(10)13/h3-6,13H,2,7-9H2,1H3
InchiKey: WOQCBCOZVWYLKS-UHFFFAOYSA-N
Formula: C12H16O3
SMILES: CCCOC(=O)CCc1ccccc1O
Mol. weight [g/mol]: 208.25
CAS: 59116-13-1

Physical Properties

Property code	Value	Unit	Source
gf	-225.97	kJ/mol	Joback Method
hf	-476.59	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.278		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1598.90		NIST Webbook
tb	657.55	K	Joback Method
tc	873.24	K	Joback Method
tf	435.30	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.08	J/mol×K	657.55	Joback Method
cpg	461.57	J/mol×K	693.50	Joback Method
cpg	474.24	J/mol×K	729.45	Joback Method
cpg	486.16	J/mol×K	765.40	Joback Method
cpg	497.38	J/mol×K	801.34	Joback Method
cpg	507.98	J/mol×K	837.29	Joback Method
cpg	518.02	J/mol×K	873.24	Joback Method
dvisc	0.0006064	Pa×s	435.30	Joback Method

dvisc	0.0002767	Pa×s	472.34	Joback Method
dvisc	0.0001415	Pa×s	509.38	Joback Method
dvisc	0.0000793	Pa×s	546.42	Joback Method
dvisc	0.0000478	Pa×s	583.47	Joback Method
dvisc	0.0000306	Pa×s	620.51	Joback Method
dvisc	0.0000206	Pa×s	657.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59116131&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