2-Monobenzoylglycerol

Inchi: InChI=1S/C10H12O4/c11-6-9(7-12)14-10(13)8-4-2-1-3-5-8/h1-5,9,11-12H,6-7H2
InchiKey: XNUZWIXOUNSBLL-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: O=C(OC(CO)CO)c1ccccc1
Mol. weight [g/mol]: 196.20
CAS: 26699-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-364.27	kJ/mol	Joback Method
hf	-567.74	kJ/mol	Joback Method
hfus	23.14	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	0.197		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
tb	715.09	K	Joback Method
tc	907.58	K	Joback Method
tf	407.68	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.93	J/mol×K	715.09	Joback Method
cpg	446.13	J/mol×K	907.58	Joback Method
cpg	439.62	J/mol×K	875.50	Joback Method
cpg	432.60	J/mol×K	843.42	Joback Method
cpg	425.03	J/mol×K	811.34	Joback Method
cpg	416.91	J/mol×K	779.25	Joback Method
cpg	408.22	J/mol×K	747.17	Joback Method
cps	236.40	J/mol×K	298.00	NIST Webbook
dvisc	0.0000111	Pa×s	715.09	Joback Method

dvisc	0.0000193	Pa×s	663.86	Joback Method
dvisc	0.0000369	Pa×s	612.62	Joback Method
dvisc	0.0000793	Pa×s	561.38	Joback Method
dvisc	0.0001985	Pa×s	510.15	Joback Method
dvisc	0.0006102	Pa×s	458.92	Joback Method
dvisc	0.0024871	Pa×s	407.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26699730&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume