1-Monobenzoylglycerol

Inchi: InChI=1S/C10H12O4/c11-6-9(12)7-14-10(13)8-4-2-1-3-5-8/h1-5,9,11-12H,6-7H2
InchiKey: SFCPXHKCMRZQAC-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: O=C(OCC(O)CO)c1ccccc1
Mol. weight [g/mol]: 196.20
CAS: 3376-59-8

Physical Properties

Property code	Value	Unit	Source
chs	-4872.70 ± 1.10	kJ/mol	NIST Webbook
gf	-364.27	kJ/mol	Joback Method
hf	-567.74	kJ/mol	Joback Method
hfs	-777.40 ± 1.20	kJ/mol	NIST Webbook
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	238.90	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=C3376598&Units=SI

Legend

chs: Standard solid enthalpy of combustion
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
hfs: Solid phase 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

Latest version available from: