Benzeneacetic acid, «alpha»-methyl-, methyl ester

Other names: Methyl hydratropate
Hydratropic acid, methyl
Methyl 2-phenylpropionate

Inchi: InChI=1S/C10H12O2/c1-8(10(11)12-2)9-6-4-3-5-7-9/h3-8H,1-2H3

InchiKey: DZIQUZJSNSZOCH-UHFFFAOYSA-N

Formula: C10H12O2

SMILES: COC(=O)C(C)c1ccccc1

Mol. weight [g/mol]: 164.20

CAS: 31508-44-8

Physical Properties

Property code	Value	Unit	Source
gf	-90.63	kJ/mol	Joback Method
hf	-263.28	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	62.00 ± 0.70	kJ/mol	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.963		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1185.00		NIST Webbook
tb	530.73	K	Joback Method
tc	748.19	K	Joback Method
tf	286.04	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.90	J/mol×K	748.19	Joback Method
cpg	300.78	J/mol×K	530.73	Joback Method
cpg	314.76	J/mol×K	566.97	Joback Method

cpg	327.92	J/mol×K	603.22	Joback Method
cpg	340.30	J/mol×K	639.46	Joback Method
cpg	351.91	J/mol×K	675.70	Joback Method
cpg	362.77	J/mol×K	711.95	Joback Method
dvisc	0.0002037	Pa×s	530.73	Joback Method
dvisc	0.0031130	Pa×s	286.04	Joback Method
dvisc	0.0014883	Pa×s	326.82	Joback Method
dvisc	0.0008382	Pa×s	367.60	Joback Method
dvisc	0.0005294	Pa×s	408.38	Joback Method
dvisc	0.0003634	Pa×s	449.17	Joback Method
dvisc	0.0002656	Pa×s	489.95	Joback Method
hvapt	61.80 ± 0.70	kJ/mol	301.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31508448&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
hvapt: Enthalpy of vaporization at a given temperature
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