4-Isobutylbenzoic acid, methyl

Inchi: InChI=1S/C12H16O2/c1-9(2)8-10-4-6-11(7-5-10)12(13)14-3/h4-7,9H,8H2,1-3H3
InchiKey: RKGMWMARQCXWPC-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: COC(=O)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-83.42	kJ/mol	Joback Method
hf	-316.03	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.672		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1443.00		NIST Webbook
tb	581.47	K	Joback Method
tc	792.78	K	Joback Method
tf	321.10	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.16	J/mol×K	581.47	Joback Method
cpg	409.45	J/mol×K	616.69	Joback Method
cpg	423.89	J/mol×K	651.91	Joback Method
cpg	437.50	J/mol×K	687.12	Joback Method
cpg	450.30	J/mol×K	722.34	Joback Method
cpg	462.32	J/mol×K	757.56	Joback Method
cpg	473.55	J/mol×K	792.78	Joback Method
dvisc	0.0021607	Pa×s	321.10	Joback Method
dvisc	0.0010969	Pa×s	364.50	Joback Method

dvisc	0.0006432	Pa×s	407.89	Joback Method
dvisc	0.0004180	Pa×s	451.29	Joback Method
dvisc	0.0002929	Pa×s	494.68	Joback Method
dvisc	0.0002174	Pa×s	538.08	Joback Method
dvisc	0.0001687	Pa×s	581.47	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=R399554&Units=SI

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