Isobutyric acid, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C12H16O2/c1-8(2)12(13)14-11-7-5-6-9(3)10(11)4/h5-8H,1-4H3
InchiKey: HXKJOHRJWKYBNW-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1cccc(OC(=O)C(C)C)c1C
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-93.05	kJ/mol	Joback Method
hf	-327.50	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	54.67	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.865		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	586.45	K	Joback Method
tc	798.75	K	Joback Method
tf	333.62	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.82	J/mol×K	586.45	Joback Method
cpg	408.86	J/mol×K	621.83	Joback Method
cpg	423.09	J/mol×K	657.22	Joback Method
cpg	436.53	J/mol×K	692.60	Joback Method
cpg	449.20	J/mol×K	727.98	Joback Method
cpg	461.11	J/mol×K	763.37	Joback Method
cpg	472.25	J/mol×K	798.75	Joback Method
dvisc	0.0016439	Pa×s	333.62	Joback Method

dvisc	0.0009045	Pa×s	375.76	Joback Method
dvisc	0.0005614	Pa×s	417.90	Joback Method
dvisc	0.0003803	Pa×s	460.04	Joback Method
dvisc	0.0002750	Pa×s	502.17	Joback Method
dvisc	0.0002091	Pa×s	544.31	Joback Method
dvisc	0.0001653	Pa×s	586.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354638&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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