

2-(4-Isobutyrylphenyl)propanoic acid, methyl

Inchi:	InChI=1S/C14H18O3/c1-9(2)13(15)12-7-5-11(6-8-12)10(3)14(16)17-4/h5-10H,1-4H3
InchiKey:	DWRCPULQORBTIR-UHFFFAOYSA-N
Formula:	C14H18O3
SMILES:	COC(=O)C(C)c1ccc(C(=O)C(C)C)cc1
Mol. weight [g/mol]:	234.29

Physical Properties

Property code	Value	Unit	Source
gf	-197.94	kJ/mol	Joback Method
hf	-475.17	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.802		Crippen Method
mvol	193.370	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	680.66	K	Joback Method
tc	896.03	K	Joback Method
tf	378.57	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.49	J/molxK	680.66	Joback Method
cpg	581.29	J/molxK	860.14	Joback Method
cpg	569.81	J/molxK	824.24	Joback Method
cpg	557.42	J/molxK	788.35	Joback Method
cpg	544.08	J/molxK	752.45	Joback Method
cpg	529.78	J/molxK	716.56	Joback Method
cpg	591.86	J/molxK	896.03	Joback Method
dvisc	0.0001314	Paxs	680.66	Joback Method

dvisc	0.0001722	Paxs	630.31	Joback Method
dvisc	0.0002364	Paxs	579.96	Joback Method
dvisc	0.0003447	Paxs	529.62	Joback Method
dvisc	0.0005441	Paxs	479.27	Joback Method
dvisc	0.0009559	Paxs	428.92	Joback Method
dvisc	0.0019510	Paxs	378.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R399529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ 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

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