4-Isopropylphenylacetic acid

Other names: p-Isopropyl phenyl acetic acid
Benzeneacetic acid, 4-(1-methylethyl)-
Inchi: InChI=1S/C11H14O2/c1-8(2)10-5-3-9(4-6-10)7-11(12)13/h3-6,8H,7H2,1-2H3,(H,12,13)
InchiKey: RERBQXVRXYCGLT-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC(C)c1ccc(CC(=O)O)cc1
Mol. weight [g/mol]: 178.23
CAS: 4476-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-123.66	kJ/mol	Joback Method
hf	-315.40	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.437		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	628.35	K	Joback Method
tc	830.56	K	Joback Method
tf	348.42	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.11	J/mol×K	628.35	Joback Method
cpg	387.20	J/mol×K	662.05	Joback Method
cpg	398.56	J/mol×K	695.75	Joback Method
cpg	409.25	J/mol×K	729.46	Joback Method
cpg	419.27	J/mol×K	763.16	Joback Method

cpg	428.66	J/mol×K	796.86	Joback Method
cpg	437.45	J/mol×K	830.56	Joback Method
dvisc	0.0050073	Pa×s	348.42	Joback Method
dvisc	0.0016186	Pa×s	395.07	Joback Method
dvisc	0.0006642	Pa×s	441.73	Joback Method
dvisc	0.0003231	Pa×s	488.38	Joback Method
dvisc	0.0001782	Pa×s	535.04	Joback Method
dvisc	0.0001082	Pa×s	581.69	Joback Method
dvisc	0.0000707	Pa×s	628.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4476282&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
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