

3-(2-Methylphenyl)propionic acid

Inchi:	InChI=1S/C10H12O2/c1-8-4-2-3-5-9(8)6-7-10(11)12/h2-5H,6-7H2,1H3,(H,11,12)
InchiKey:	JIRKNEAMPYVPTD-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	Cc1ccccc1CCC(=O)O
Mol. weight [g/mol]:	164.20
CAS:	22084-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-129.64	kJ/mol	Joback Method
hf	-289.48	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.012		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	605.91	K	Joback Method
tc	807.12	K	Joback Method
tf	352.15	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.71	J/molxK	605.91	Joback Method
cpg	375.96	J/molxK	773.59	Joback Method
cpg	367.30	J/molxK	740.05	Joback Method
cpg	358.07	J/molxK	706.52	Joback Method
cpg	348.25	J/molxK	672.98	Joback Method
cpg	337.80	J/molxK	639.45	Joback Method
cpg	384.07	J/molxK	807.12	Joback Method
dvisc	0.0000889	Paxs	605.91	Joback Method
dvisc	0.0001322	Paxs	563.62	Joback Method

dvisc	0.0002095	Paxs	521.32	Joback Method
dvisc	0.0003602	Paxs	479.03	Joback Method
dvisc	0.0006879	Paxs	436.74	Joback Method
dvisc	0.0015091	Paxs	394.44	Joback Method
dvisc	0.0039982	Paxs	352.15	Joback Method

Sources

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=C22084895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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