3-(2-Methoxyphenyl)propionic acid

Other names:	o-Methoxyhydrocinnamic acid
	2-Methoxyhydrocinnamic acid
	3-(o-Methoxyphenyl)propionic acid
	Benzenepropanoic acid, 2-methoxy-
	Benzenpropionic acid, 2-methoxy
Inchi:	InChI=1S/C10H12O3/c1-13-9-5-3-2-4-8(9)6-7-10(11)12/h2-5H,6-7H2,1H3,(H,11,12)
InchiKey:	XSZSNLOPIWWFHS-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccccc1CCC(=O)O
Mol. weight [g/mol]:	180.20
CAS:	6342-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-234.64	kJ/mol	Joback Method
hf	-421.70	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hsub	117.80 ± 1.40	kJ/mol	NIST Webbook
hvap	66.63	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.712		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	628.33	K	Joback Method
tc	827.77	K	Joback Method
tf	374.38	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.96	J/mol×K	827.77	Joback Method
cpg	350.22	J/mol×K	628.33	Joback Method
cpg	361.17	J/mol×K	661.57	Joback Method

cpg	371.50	J/mol×K	694.81	Joback Method
cpg	381.24	J/mol×K	728.05	Joback Method
cpg	390.39	J/mol×K	761.29	Joback Method
cpg	398.96	J/mol×K	794.53	Joback Method
dvisc	0.0000667	Pa×s	628.33	Joback Method
dvisc	0.0024094	Pa×s	374.38	Joback Method
dvisc	0.0009783	Pa×s	416.70	Joback Method
dvisc	0.0004691	Pa×s	459.03	Joback Method
dvisc	0.0002546	Pa×s	501.35	Joback Method
dvisc	0.0001520	Pa×s	543.68	Joback Method
dvisc	0.0000978	Pa×s	586.00	Joback Method
hfust	25.33	kJ/mol	360.50	NIST Webbook
hsubt	116.00 ± 0.40	kJ/mol	339.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6342774&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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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