Benzenebutanoic acid, 2,5-dimethyl-

Other names: Butyric acid, 4-(2,5-xylyl)-
«gamma»-(2,5-Dimethylphenyl)-n-butyric acid
4-(2,5-Xylyl)butanoic acid
Inchi: InChI=1S/C12H16O2/c1-9-6-7-10(2)11(8-9)4-3-5-12(13)14/h6-8H,3-5H2,1-2H3,(H,13,14)
InchiKey: XNTQOUBHYSKYOI-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1ccc(C)c(CCCC(=O)O)c1
Mol. weight [g/mol]: 192.25
CAS: 1453-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-122.43	kJ/mol	Joback Method
hf	-342.23	kJ/mol	Joback Method
hfus	25.79	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.711		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	656.65	K	Joback Method
tc	853.59	K	Joback Method
tf	387.21	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.11	J/mol×K	656.65	Joback Method
cpg	435.41	J/mol×K	689.47	Joback Method
cpg	447.04	J/mol×K	722.30	Joback Method
cpg	458.01	J/mol×K	755.12	Joback Method
cpg	468.35	J/mol×K	787.94	Joback Method
cpg	478.08	J/mol×K	820.76	Joback Method

cpg	487.23	J/mol×K	853.59	Joback Method
dvisc	0.0021614	Pa×s	387.21	Joback Method
dvisc	0.0008826	Pa×s	432.12	Joback Method
dvisc	0.0004266	Pa×s	477.02	Joback Method
dvisc	0.0002337	Pa×s	521.93	Joback Method
dvisc	0.0001408	Pa×s	566.84	Joback Method
dvisc	0.0000914	Pa×s	611.74	Joback Method
dvisc	0.0000629	Pa×s	656.65	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1453061&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume