Butyric acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C12H16O2/c1-4-5-12(13)14-11-7-9(2)6-10(3)8-11/h6-8H,4-5H2,1-3H3
InchiKey: ARQBYJXHHMRZOF-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-90.61	kJ/mol	Joback Method
hf	-322.22	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.009		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	586.89	K	Joback Method
tc	794.87	K	Joback Method
tf	348.62	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.42	J/mol×K	586.89	Joback Method
cpg	459.32	J/mol×K	760.20	Joback Method
cpg	447.61	J/mol×K	725.54	Joback Method
cpg	435.18	J/mol×K	690.88	Joback Method
cpg	422.01	J/mol×K	656.22	Joback Method
cpg	408.10	J/mol×K	621.55	Joback Method
cpg	470.31	J/mol×K	794.87	Joback Method
dvisc	0.0001769	Pa×s	586.89	Joback Method

dvisc	0.0002193	Pa×s	547.18	Joback Method
dvisc	0.0002812	Pa×s	507.47	Joback Method
dvisc	0.0003763	Pa×s	467.75	Joback Method
dvisc	0.0005313	Pa×s	428.04	Joback Method
dvisc	0.0008050	Pa×s	388.33	Joback Method
dvisc	0.0013410	Pa×s	348.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307514&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
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