Nonanoic acid, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C17H26O2/c1-4-5-6-7-8-9-13-17(18)19-16-12-10-11-14(2)15(16)3/h10-12H,4-9
InchiKey: QCWAARQRPVKNFR-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-48.51	kJ/mol	Joback Method
hf	-425.42	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.959		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2013.00		NIST Webbook
tb	701.29	K	Joback Method
tc	896.38	K	Joback Method
tf	404.97	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.31	J/mol×K	701.29	Joback Method
cpg	671.53	J/mol×K	733.80	Joback Method
cpg	687.82	J/mol×K	766.32	Joback Method
cpg	703.19	J/mol×K	798.83	Joback Method
cpg	717.67	J/mol×K	831.35	Joback Method
cpg	731.28	J/mol×K	863.86	Joback Method
cpg	744.04	J/mol×K	896.38	Joback Method
dvisc	0.0010807	Pa×s	404.97	Joback Method
dvisc	0.0005971	Pa×s	454.36	Joback Method

dvisc	0.0003706	Pa×s	503.74	Joback Method
dvisc	0.0002505	Pa×s	553.13	Joback Method
dvisc	0.0001805	Pa×s	602.52	Joback Method
dvisc	0.0001367	Pa×s	651.90	Joback Method
dvisc	0.0001077	Pa×s	701.29	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360671&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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