Dodecanoic acid, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C20H32O2/c1-4-5-6-7-8-9-10-11-12-16-20(21)22-19-15-13-14-17(2)18(19)3/h1
InchiKey: FGJCENRKFKUYPW-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	-23.25	kJ/mol	Joback Method
hf	-487.34	kJ/mol	Joback Method
hfus	43.61	kJ/mol	Joback Method
hvap	72.87	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.130		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	2332.00		NIST Webbook
tb	769.93	K	Joback Method
tc	962.18	K	Joback Method
tf	438.78	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.82	J/mol×K	769.93	Joback Method
cpg	906.31	J/mol×K	930.14	Joback Method
cpg	892.15	J/mol×K	898.10	Joback Method
cpg	877.05	J/mol×K	866.06	Joback Method
cpg	860.97	J/mol×K	834.01	Joback Method
cpg	843.91	J/mol×K	801.97	Joback Method
cpg	919.56	J/mol×K	962.18	Joback Method
dvisc	0.0000749	Pa×s	769.93	Joback Method
dvisc	0.0000962	Pa×s	714.74	Joback Method

dvisc	0.0001289	Pa×s	659.55	Joback Method
dvisc	0.0001820	Pa×s	604.36	Joback Method
dvisc	0.0002754	Pa×s	549.16	Joback Method
dvisc	0.0004574	Pa×s	493.97	Joback Method
dvisc	0.0008629	Pa×s	438.78	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=U360547&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