Octanoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C16H24O2/c1-4-5-6-7-8-9-16(17)18-15-11-13(2)10-14(3)12-15/h10-12H,4-9H2
InchiKey: WQSWUBODLKASOP-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-56.93	kJ/mol	Joback Method
hf	-404.78	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.569		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	678.41	K	Joback Method
tc	875.38	K	Joback Method
tf	393.70	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.40	J/mol×K	678.41	Joback Method
cpg	674.82	J/mol×K	842.55	Joback Method
cpg	661.47	J/mol×K	809.73	Joback Method
cpg	647.27	J/mol×K	776.90	Joback Method
cpg	632.21	J/mol×K	744.07	Joback Method
cpg	616.26	J/mol×K	711.24	Joback Method
cpg	687.35	J/mol×K	875.38	Joback Method
dvisc	0.0001204	Pa×s	678.41	Joback Method

dvisc	0.0001522	Pa×s	630.96	Joback Method
dvisc	0.0002000	Pa×s	583.51	Joback Method
dvisc	0.0002756	Pa×s	536.05	Joback Method
dvisc	0.0004044	Pa×s	488.60	Joback Method
dvisc	0.0006444	Pa×s	441.15	Joback Method
dvisc	0.0011489	Pa×s	393.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307696&Units=SI

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