Methyl 3,5-di-t-butylsalicylate

Other names: Methyl 3,5-di-tert-butylsalicylate
Inchi: InChI=1S/C16H24O3/c1-15(2,3)10-8-11(14(18)19-7)13(17)12(9-10)16(4,5)6/h8-9,17H,1-
InchiKey: QSGONIQEKLJPGV-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: COC(=O)c1cc(C(C)(C)C)cc(C(C)(C)C)c1O
Mol. weight [g/mol]: 264.36
CAS: 15018-03-8

Physical Properties

Property code	Value	Unit	Source
gf	-205.87	kJ/mol	Joback Method
hf	-599.59	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.774		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
tb	752.57	K	Joback Method
tc	978.28	K	Joback Method
tf	510.26	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.31	J/mol×K	752.57	Joback Method
cpg	678.30	J/mol×K	790.19	Joback Method
cpg	693.33	J/mol×K	827.81	Joback Method
cpg	707.50	J/mol×K	865.42	Joback Method
cpg	720.95	J/mol×K	903.04	Joback Method
cpg	733.78	J/mol×K	940.66	Joback Method
cpg	746.11	J/mol×K	978.28	Joback Method
dvisc	0.0001455	Pa×s	510.26	Joback Method

dvisc	0.0000698	Pa×s	550.64	Joback Method
dvisc	0.0000370	Pa×s	591.03	Joback Method
dvisc	0.0000213	Pa×s	631.41	Joback Method
dvisc	0.0000131	Pa×s	671.80	Joback Method
dvisc	0.0000085	Pa×s	712.19	Joback Method
dvisc	0.0000058	Pa×s	752.57	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=C15018038&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume