2,4,6-TRIISOPROPYLBENZOIC ACID

Other names: Benzoic acid, 2,4,6-tris(1-methylethyl)-
2,4,6-tris(1-methylethyl)benzoic acid
Inchi: InChI=1S/C16H24O2/c1-9(2)12-7-13(10(3)4)15(16(17)18)14(8-12)11(5)6/h7-11H,1-6H3,
InchiKey: ULVHAZFBJJXIDO-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CC(C)c1cc(C(C)C)c(C(=O)O)c(C(C)C)c1
Mol. weight [g/mol]: 248.37

Physical Properties

Property code	Value	Unit	Source
hf	-511.73	kJ/mol	Cheméo Relay (1.0)
hfus	25.19	kJ/mol	Joback Method
hvap	98.10	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
logp	4.755		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
tb	562.43	K	Cheméo Relay (1.0)
tf	384.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.37	J/mol×K	751.83	Joback Method
cpg	711.98	J/mol×K	951.40	Joback Method
cpg	701.20	J/mol×K	918.14	Joback Method
cpg	689.66	J/mol×K	884.88	Joback Method
cpg	677.34	J/mol×K	851.61	Joback Method
cpg	664.20	J/mol×K	818.35	Joback Method
cpg	650.22	J/mol×K	785.09	Joback Method
dvisc	0.0001179	Pa×s	575.82	Joback Method
dvisc	0.0000254	Pa×s	751.83	Joback Method
dvisc	0.0000389	Pa×s	693.16	Joback Method
dvisc	0.0000643	Pa×s	634.49	Joback Method
dvisc	0.0021146	Pa×s	399.81	Joback Method

dvisc	0.0002481	Pa×s	517.15	Joback Method
dvisc	0.0006315	Pa×s	458.48	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49623714&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point