Methyl 3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]pro

Other names: Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate
Methylox

Inchi: InChI=1S/C18H28O3/c1-17(2,3)13-10-12(8-9-15(19)21-7)11-14(16(13)20)18(4,5)6/h10-1

InchiKey: PXMJCECEFTYEKE-UHFFFAOYSA-N

Formula: C18H28O3

SMILES: COC(=O)CCc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1

Mol. weight [g/mol]: 292.42

Physical Properties

Property code	Value	Unit	Source
hf	-661.51	kJ/mol	Cheméo Relay (1.0)
hfus	29.38	kJ/mol	Joback Method
hvap	99.78	kJ/mol	Cheméo Relay (1.0)
ie	7.78	eV	Cheméo Relay (1.0)
logp	4.093		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1943.30		NIST Webbook
rinpol	1943.30		NIST Webbook
tb	575.95	K	Cheméo Relay (1.0)
tf	359.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.27	J/mol×K	798.33	Joback Method
cpg	790.89	J/mol×K	834.92	Joback Method
cpg	806.61	J/mol×K	871.50	Joback Method
cpg	821.52	J/mol×K	908.09	Joback Method
cpg	835.75	J/mol×K	944.67	Joback Method
cpg	849.42	J/mol×K	981.26	Joback Method
cpg	862.62	J/mol×K	1017.84	Joback Method
dvisc	0.0001008	Pa×s	532.80	Joback Method
dvisc	0.0000470	Pa×s	577.05	Joback Method

dvisc	0.0000244	Pa×s	621.31	Joback Method
dvisc	0.0000139	Pa×s	665.57	Joback Method
dvisc	0.0000084	Pa×s	709.82	Joback Method
dvisc	0.0000054	Pa×s	754.08	Joback Method
dvisc	0.0000037	Pa×s	798.33	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6386385&Units=SI

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

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
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point