

Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester

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]:	292.41
CAS:	6386-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-189.03	kJ/mol	Joback Method
hf	-640.87	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	78.84	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
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	798.33	K	Joback Method
tc	1017.84	K	Joback Method
tf	532.80	K	Joback Method
vc	0.903	m3/kmol	Joback Method

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

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=C6386385&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

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